CO₂QUEST | **IoLiCAP**

INTERNATIONAL FORUM ON RECENT DEVELOPMENTS OF CCS IMPLEMENTATION
LEADING THE WAY TO A LOW-CARBON FUTURE

26TH - 27TH MARCH, 2015

ATHENS, GREECE

ATHENS LEDRA HOTEL

DELEGATE PACK

WELCOME

Dear Esteemed Participants and Attendees,

As coordinators of the co-organising E.C. FP7 Projects, CO_2QUEST and IoLiCAP, we would like to thank you for attending the INTERNATIONAL FORUM ON RECENT DEVELOPMENTS OF CCS IMPLEMENTATION.

The Forum covers all the important aspects of the CCS chain, presenting the latest findings of several European and international projects whose research is critical to the development of safe and economically viable CCS technologies. The event brings together key players in academia, research institutions, industry stakeholders and the European Commission, thus forming a unique knowledge-sharing experience for all.

In-line with the multidisciplinary nature of CCS, we have organized eight different sessions covering: combustion, including chemical looping for gaseous fuels; new solvents and materials for CO_2 capture; transport and safety; storage-monitoring and safety; molecular simulation and design of new solvents and materials; thermodynamic modelling; thermophysical properties; corrosion protection and monitoring; integration and techno-economic studies; environmental impact assessment; waste management; public acceptance; and the European and International markets.

We would also like to thank the members of the Organising Committee, especially Ms. Abigail Ward, Dr. Robert Woolley and Prof. Ioannis Economou for their hard work and excellent organisation of this important international gathering.

We hope you enjoy attending the technical sessions and find the opportunity for fruitful future collaborations and knowledge exchange.

Prof. Haroun Mahgerefteh   Dr. George Romanos
CO2QUEST FP7 Project Coordinator   IoLiCAP FP7 Project Coordinator
       http://www.co2quest.eu/   http://www.iolicap.eu/

THE ORGANISING COMMITTEE

Co-chair: Dr. Robert M. Woolley – University of Leeds, UK

Co-chair: Dr. George Romanos – National Center for Scientific Research "Demokritos", Greece

Member: Prof. Ioannis G. Economou - Texas A&M University at Qatar

Member: Miss Abigail Ward – University of Leeds, UK

Member: Dr. Niall Mac Dowell - Imperial College London, UK

Member: Dr. Sergey Martynov - University College London, UK

WITH SPECIAL THANKS TO

INTRODUCING THE KEYNOTE SPEAKERS

DR. VASSILIOS KOUGIONAS (DG RESEARCH & INNOVATION, EC)

Dr. Vassilios Kougionas holds a PhD in Chemical Reaction Engineering from Imperial College, London, a Bachelors degree in Petrochemical Engineering from University of London, and a Master's of Science in Advanced Chemical Engineering. In addition, Dr. Kougionas has received a Master's in Business Administration from Solvay Management School Brussels.

Dr. Kougionas worked as a Senior Research Fellow at Imperial College London, as a Senior Research Engineer at C.N.R.S. Institute of Catalysis in Lyon, France and as a Senior Researcher and Lecturer at the National Technical University of Athens.

In 1998, Dr. Kougionas joined the European Commission, Directorate General for Energy in Brussels where he worked for six years as a sector leader for research and development of Conventional Energies from Oil, Gas and Coal.

Since 2004, he has worked at the European Commission Directorate General for Research in the Energy Directorate, being responsible for Fossils Fuels, Carbon Capture and Storage and International Cooperation Issues. He is the desk officer for the Commission for the European Zero Emission Power (ZEP) Technology Platform and a delegate at the IEA Working Party of Fossil Fuels.

DR. PAUL FENNELL (ICL, UK)

Dr. Paul Fennell is a Reader in Clean Energy at Imperial College London. He obtained his degree in Chemical Engineering and PhD from the University of Cambridge. He chairs the Institution of Chemical Engineers Energy Conversion subject panel, was a previous member of the International Energy Authority High-Temperature Solid Looping Cycles Network Executive, and has written reports for the Department for Energy and Climate Change (DECC) on future technologies for Carbon Capture and Storage (CCS) and carbon capture readiness. Dr. Fennell is also the joint director of Imperial College's Centre for Carbon Capture and Storage and is the Research Area Champion for Industrial CO_2 Capture and Storage for the UK CO_2 Capture and Storage Research Centre. He has published over 50 academic papers since 2005 and is the 2015 winner of the Institution of Chemical Engineers' Ambassador prize.

MR. JOHN GALE (IEA GREENHOUSE GAS R&D)

Mr. John Gale is the General Manager of the IEA Greenhouse Gas R&D Programme (IEAGHG), an Implementing Agreement established under the IEA in 1991. The IEAGHG is an international non-profit organisation that undertakes research on the mitigation of greenhouse gas emissions from fossil fuel use. In recent years its research activities have focused largely upon carbon capture and storage CCS. Mr. Gale acts as the IEAGHG representative on the Steering Committees for the Greenhouse Gas Control Technology conferences (GHGT). The GHGT conference series has established itself as the premier international technical conference on CCS in the world. In addition to his role with IEAGHG Mr. Gale is the Editor in Chief of the International Journal of Greenhouse Gas Control published by Elsevier. Mr. Gale sits on various technical committees within the IEA and elsewhere and is currently the Chair of the Independent Advisory Panel for the UKCCSRC.

MR. RUSSELL COOPER (NATIONAL GRID, UK)

Mr. Russell Cooper is the technical lead for Carbon Capture and Storage within National Grid and has 25 years' experience in various planning and asset management roles in National Grid.

Mr. Cooper leads both the onshore and offshore developments for the Humber transport and storage scheme. This development of a network solution and large offshore aquifer storage is capable of receiving large quantities of Carbon Dioxide (CO_2) from multiple emitters including the Don Valley and White Rose projects. This leading edge development is in an advanced planning stage, having been formally notified to the Planning Inspectorate and with extensive public engagement already completed.

Mr. Cooper is heavily involved in developing research associated with transportation of Carbon Dioxide. He is a board member of the UKCCS Research Council. Mr. Cooper has also led the development of in-house National Grid research, intended to deliver the safe design of high pressure Carbon Dioxide pipelines.

Mr. Cooper was National Grids technical lead for the DECC-1 Front End Engineering and Design (FEED) study conducted on the Longannet power station CCS project, which proved the reuse of existing pipeline assets for CO_2 transportation.

AGENDA

THURSDAY, 26 MARCH, 2015		
08:30	**Registration / Welcome coffee**	Pre-function area
09:00	**Opening: Welcome and Introduction** Dr. Robert M. Woolley (University of Leeds, UK)	Aegina/Hydra/Spetses meeting room
09:05	**Opening Remarks: CO2QUEST P.I.** Prof. Haroun Mahgerefteh (UCL, UK)	
09:10	**Plenary Lecture 1: Update from the European Commission Initiatives on CCS from the Research and Innovation Perspective** Dr. Vassilios Kougionas (DG Research & Innovation, EC) **Chair: Prof. Haroun Mahgerefteh (UCL, UK)**	
Session 1: Transport and Safety 1 **Chair: Prof. Haroun Mahgerefteh (UCL, UK)**		
10:00	**Numerical Modelling of Heat Transfer Phenomena in Accidental CO_2 Pipeline Release Scenarios** Robert Woolley (University of Leeds, UK)	
10:20	**Predicting the Atmospheric Dispersion of Carbon Dioxide Releases from Pipelines for CCS Applications using CO2FOAM** Jennifer Wen (University of Warwick, UK)	
10:40	**A Study of Transient Two-phase Flows in CO_2 Pipelines** Solomon Brown (UCL, UK)	
11:00	**Measurement of Water Solubility Limits in CO_2 Mixtures to Ensure the Safe Pipeline Transportation of CO_2** Stephanie Foltran (University of Nottingham, UK)	
11:20	**COFFEE BREAK**	Pre-function area
Session 2: Capture 1 **Chair: Dr. George Romanos (NCSRD, Greece)**		
11:40	**CO_2 Capture by Novel Supported Ionic Liquid Phase Materials Consisting of Silica Encapsulated Chitosan Ionogels** Peter Schultz (University of Erlangen, Germany)	Aegina/Hydra/Spetses meeting room
12:00	**Optimised PEI impregnation of Activated Carbons - Enhancement of Post-combustion CO_2 Capture** Antonio Salituro (University of Leeds, UK)	
12:20	**Molecular Simulation of Ionic Liquid Solvents for CO_2 Capture** Niki Vergadou (NCSRD, Greece)	

12:40	**LUNCH**	Zephyros Restaurant
13:30	**Plenary Lecture 2: Comparative Costings for 1st, 2nd and 3rd Generation CCS technologies** Dr. Paul Fennell (ICL, UK) **Chair: Dr. Niall Mac Dowell (ICL, UK)**	Aegina/Hydra/Spetses meeting room
Session 3: Process Optimisation and Techno-economic Considerations **Chair: Dr. Niall Mac Dowell (ICL, UK)**		
14:20	**Computationally Efficient Surrogate Based Multi-objective Optimisation for Pressure Swing Adsorption for Carbon capture** Eric Fraga (UCL, UK)	
14:40	**IMPACTS: Economic Trade-offs in Establishing CO_2 Impurity Specifications** Charles Eickhoff (Progressive Energy Ltd., UK)	
15:00	**Techno-economic Analysis of Gas Purification for CO_2 Transport and Injection for Storage** Clea Kolster (ICL, UK)	
15:20	**CCS System Modelling: Enabling Technology to Help Accelerate Commercialisation and Reduce Technology Risk – A Case Study on the Operation of CCS Networks** Mario Calado (PSE, UK)	
15:40	**COFFEE BREAK**	Pre-function area
Session 4: Thermophysical Properties **Chair: Prof. Ioannis Economou (Texas A&M University, Qatar)**		
16:00	**Thermophysical Properties of Tricyanomethanide and Tetracyanoborate-Based Ionic Liquids by Using Dynamic Light Scattering and Conventional Methods** Peter Schultz (University of Erlangen, Germany)	Aegina/Hydra/Spetses meeting room
16:20	**Solubility and Kinetics of CO_2 in Low Transition Temperature Mixtures: Experiments and Modelling** Lawien Zubeir (Eindhoven University of Technology, Netherlands)	
16:40	**Measurements on Volumetric Properties of binaries and ternaries of Carbon dioxide, Nitrogen, and Argon at Supercritical State by Single Sinker Densimeter** Xiaoxian Yang (Tsinghua University, China)	
17:00	**Thermophysical Properties for Transport and Storage of CO_2-rich Mixtures – Contributions by IMPACTS** Roland Span (Ruhr-Universität Bochum, Germany)	

17:20	**Prediction of Physical Properties for CCS Process Design Using Molecular Simulation** Ioannis Economou (Texas A&M University, Qatar)	Aegina/Hydra/Spetses meeting room
17:40	**CO_2+SO_2 Co-capture Assessment. Part 1.** Sofia Blanco (University of Zaragoza, Spain)	
18:00	**Close: Notices**	

COCKTAIL DINNER
20:00 – 22:00: Cocktail dinner at the *Ledra Kai Restaurant*, located at the Ledra Hotel Athens.

	FRIDAY, 27 MARCH, 2015	
08:30	**Registration / Welcome coffee**	Pre-function area
09:00	**Opening: Welcome and Introduction by IoLiCAP P.I.** Dr. George Romanos (NCSRD, Greece)	Aegina/Hydra/Spetses meeting room
09:10	**Plenary Lecture 3: A Global Overview of CCS Implementation** Mr. John Gale (IEA Greenhouse Gas R&D) **Chair: Dr. George Romanos (NCSRD, Greece)**	
Session 5: Storage **Chair: Dr. Dorothee Rebscher (BGR, Germany)**		
10:00	**A Geochemical Database for Subsurface Applications – Theory and Experiments** Henning Peters (Shell Global Solutions, Netherlands)	
10:20	**Potential Impact of Selected Impurities on Geochemistry Related to CO_2 Storage** Dorothee Rebscher (BGR, Germany)	
10:40	**The Plains CO_2 Reduction Partnership: Demonstrating Carbon Dioxide Storage in the United States and Canada** Charles Gorecki (University of North Dakota, USA)	
11:00	**Predicting the Long Term Fate of the Stored CO_2: Main Findings of the EU-FP7 Funded PANACEA Project** Jacob Bensabat (EWRE, Israel)	
11:20	**COFFEE BREAK**	Pre-function area
Session 6: Transport and Safety 2 **Chair: Prof. Roland Span (Ruhr-Universität Bochum, Germany)**		
11:40	**Numerical Modelling of Dynamic Brittle Crack Initiation and Propagation of Pipeline Steel** Reza Talemi (OCAS, Belgium)	Aegina/Hydra/Spetses meeting room
12:00	**CO_2 Compression and Flow in Transportation Networks** Sergey Martynov (UCL, UK)	
12:20	**Impact of Impurities on Pipeline Specification and Hydraulics** Julia Race (University of Strathclyde, UK)	
12:40	**Effect of Ionic Liquids with Imidazolium and Lactam-Based Cations on Corrosion of Mild Steel** Igor Molchan (University of Manchester, UK)	
13:00	**LUNCH**	Zephyros Restaurant

13:50	**Plenary Lecture 4: Transferring CCS Research into Good Transportation Design** Mr. Russell Cooper (National Grid, UK) **Chair: Dr. Vassilios Kougionas (DG Research & Innovation, EC)**	Aegina/Hydra/Spetses meeting room
Session 7: Capture 2 **Chair: Dr. George Romanos (NCSRD, Greece)**		
14:40	**The Role of Degradation on Foaming of Various Amine Solvents in Model Columns** Kyra Campbell (ICL, UK)	
15:00	**Do Ether Functionalized Ionic Liquids Improve the CO_2 Solubility?** Lawien Zubeir (Eindhoven University of Technology, Netherlands)	
15:20	**Up-scaled Synthesis of TCM-based Ionic Liquids for CO_2 Capture** Boyan Iliev (IOLITEC, Germany)	
15:40	**On the Use of Ionic Liquids in Order to Inhibit/Promote CO_2 Hydrates** George Romanos (NCSRD, Greece)	
16:00	**COFFEE BREAK**	Pre-function area
Session 8: Combustion **Chair: Prof. Jennifer Wen (University of Warwick, UK)**		
16:20	**Gas-CCS: Experimental Impact of CO_2 Enhanced Air on Combustion Characteristics and Microturbine Performance** Thom Best (University of Leeds, UK)	Aegina/Hydra/Spetses meeting room
16:40	**Pressurised Carbonation Experiments in the Presence of Steam in a Spouted-Bed Reactor** Joseph Yao (ICL, UK)	
17:00	**Investigating the Performance of Fe-based Oxygen Carriers for Pressurised Chemical-looping Combustion of Gaseous Fuels** Zili Zhang (ICL, UK)	
17:20	**Closing Remarks** Mr. Peter Petrov, IoLiCAP Programme Officer (DG Research & Innovation, EC)	
17:30	**Close: Thanks and end of conference by CO2QUEST P.I.** Prof. Haroun Mahgerefteh (UCL, UK)	

The following posters will be presented throughout the event:

POSTERS
Investigation of the Effect of Elevation and Impurities on CO_2 Pipeline Repressurisation Distance Using Aspen Hysys 8.6V Process Simulator Victor Onyebuchi (Cranfield University, UK)
Feasibility Study of Microbial Associated CO_2 Geological Storage Atsuko Tanaka (AIST, Japan)
Technical Design of a CO_2 Transport System From Western Macedonia Power Stations to the Prinos Oil Field, Greece Alexandros Tasianas (NTUA, Greece)
Calculation of Gas Solubility in Selected Ionic Liquids and their Aqueous Solutions with ePC-SAFT Theodora Spyriouni (Scienomics, Greece)
Multi-Criteria Decision Support for Evaluating CCS Technologies Stefanie Niekamp (TWI Ltd., UK)
Effect of Cryogenic Air Separation Purity on Oxy-fuel Combustion for Carbon Capture Pedro Rivotti (ICL, UK)
A Model of the Near-field Expansion of CO_2 Jet Released from a Ruptured Pipeline Wentian Zheng (UCL, UK)
Compression Requirements for Post-combustion, Pre-Combustion and Oxy-fuel CO_2 Streams in CCS Nor Daud (UCL, UK)
Comparison of Numerical Predictions with CO_2 Pipeline Release Datasets of Relevance to CCS Applications Robert Woolley on behalf of Chris Wareing (University of Leeds, UK)
Industrial Scale CO_2 Release Experiment Facility Modelling CO_2 Pipeline Failure Richard Chen (DUT, China)
Synthesis of Selective CO_2 Sorbents for Post-combustion Capture: The Key Role of the Intrinsic Basicity Originated from Oak Wood Antonio Salituro (University of Leeds, UK)
Inside and Outside Flow from Pipes Containing a Dense CO_2 Mixture Incorporating Impurities: Experimental Set-up and First Results Jerome Hébrard (INERIS, France)
CO_2 and its Impurities Along the CCS chain : Overview of Possible Impacts and the Criteria for Risk Assessment Regis Farret (INERIS, France)

PRESENTATION ABSTRACTS

Update from the European Commission Initiatives on CCS from the Research and Innovation Perspective

V. Kougionas*[1]

*Presenting author's email: Vassilios.Kougionas@ec.europa.eu

[1] *European Commission, DG Research & Innovation, Brussels/Belgium*

Abstract

General EU energy policy framework and current progress against on the EC's projections for 2020, under its 2020 Climate and Energy Framework, before going on the more demanding 2030 projections. Summarised progress on the SET Plan, the technology pillar of EU energy and climate change policy, and an update on the Horizon 2020 programme will be given, with its budget for the period 2014 to 2020 of €79 billion.

Then a more detailed review on CCS initiatives undertaken by the European Commission will be provided to move the technology forward. Initiatives that will be covered, e.g. demonstration, communication and public engagement, knowledge sharing, legal and regulatory matters, storage capacity and infrastructure. On research and development around €220 million had been spent in Framework Programme 7 for Research and Innovation between 2007-2013 on clean coal and CCS. Priorities on CCS under Horizon 2020 including international cooperation will be provided.

Numerical modelling of turbulence and heat transfer phenomena in accidental CO$_2$ pipeline releases

R.M. Woolley*[1], M. Fairweather[1], C.J. Wareing[2] and S.A.E.G. Falle[3]

*r.m.woolley@leeds.ac.uk

[1]School of Chemical and Process Engineering, [2]School of Physics and Astronomy, and [3]School of Mathematics, University of Leeds, Leeds LS2 9JT, UK

Abstract

With the progressive development and roll-out of CCS technology in the UK, Europe, and world-wide, it is envisaged that pipeline transport of CO$_2$ will be essential in the future in order to access on- and off-shore storage sites. It is inevitable that these pipelines will, in part, pass near to populated areas, and as such, validated numerical models will be required to predict the behaviour of accidental releases in terms of phase composition and dispersion. These can subsequently be applied in risk assessment tools for the planning, construction, and operation of CO$_2$ pipelines. It has been identified that the transported fluid will be of variable composition, and contain impurities dependent upon its origin [1], which will inevitably have an impact upon the thermodynamic behaviour of the system. The CO2QUEST project, of which this work draws from, addresses the fundamentally important issues regarding the impact of the typical impurities in the gas or dense phase CO$_2$ stream captured from fossil fuel power plants on its safe and economic transportation and storage.

The numerical approach to the modelling of the under-expanded jets was based upon the solutions of the Reynolds-averaged, density-weighted forms of the transport equations for mass, momentum, and total energy as described in detail in Woolley et al. [2]. This equation set was closed by the application of a two-equation turbulence model and also a second-moment Reynolds-stress transport model. A number of turbulence sub-models have been investigated, and are referenced in Figure 1, which reports predictions of the normalized centreline axial velocity, plotted against
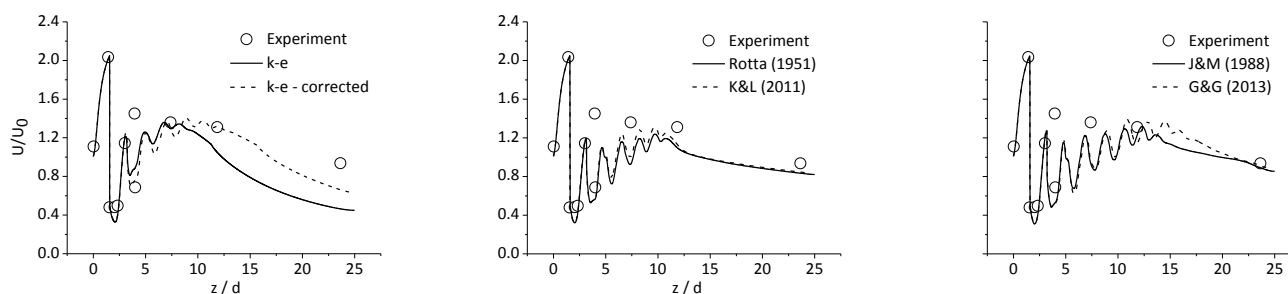

FIGURE 1.   Normalised axial velocity predictions (lines) of the highly under-expanded jet plotted against experimental data (symbols) as a function of distance normalised by the nozzle diameter (d).

experimental data for a highly under-expanded air jet [3] with a nozzle-pressure ratio of 3.57. As expected, the unmodified k-ε model over-predicts the jet mixing, leading to an over-dissipative solution. The application of a compressible turbulence dissipation rate goes some way to correcting this, as can be seen by the increase in the amplitude and more gradual decay of the decompression-compression cycle evident in the velocity curve. The resolution of the initial shock-laden region remains poor however, and the solution subsequently becomes overly dissipative with downstream progression. The Reynolds-stress transport model with the closure of the pressure-strain correlation attributed to Rotta [4] notably improves upon the resolution of the shock region and the prediction of the dissipation of turbulence kinetic energy. The introduction of a compressible element to the 'slow' part of the model as discussed by Khlifi and Lili [5] effects an additional increase in peak magnitude predictions in the near field, although has little effect upon the subsequent downstream dissipation. Application of a model for the 'rapid' part of the pressure-strain term [6], incorporated with the model of Rotta for the 'slow' part is a significant improvement with respect to predictions of the shock resolution and the turbulence dissipation. This is again improved by the introduction of corrections based upon the turbulent and gradient Mach numbers reported by Gomez and Girimaji [7].
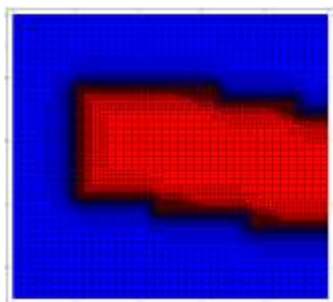
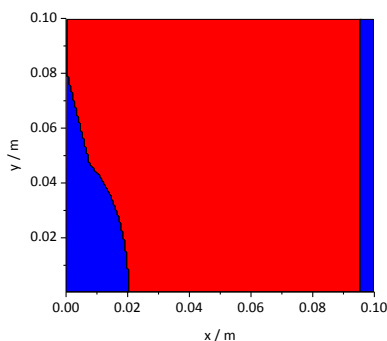Figure 3. Example of adaptive mesh refinement in the location of the crack.

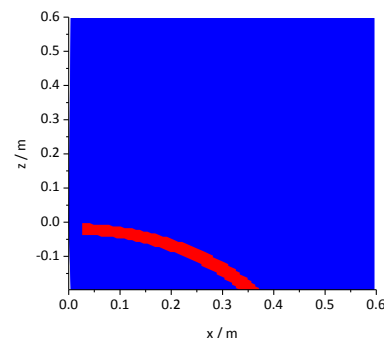Figure 4. Modelled crack geometry showing two-planar axisymmetry.

Figure 5. Cross-sectional view of the three- dimensional domain.

The near-field release model is capable of predicting the thermophysical behaviour of releases in any complex geometry described, and Figure 4 shows a plan view of a sample geometry of a puncture and pre-formed crack, extending in the axial direction of the pipe. This was incorporated into a three-dimensional model in which one quarter of the crack has been modelled by applying the appropriate symmetry boundaries on the x and y planes. The three-dimensional domain extends 0.6 meters above the release plane, and in the direction of the expansion radius. This is to accommodate the expansion zone of the release, including phenomena such as the shock front. Figure 5 depicts this domain on the y=0 plane, providing a cross-sectional view of the release pipe and the crack centre. Figure 3 shows an example of the adaptive mesh located at the crack edge, in the geometry of Figure 5. There are levels of refinement, with the highest density of control volumes located at the interface between the pipe wall and the surrounding fluid.
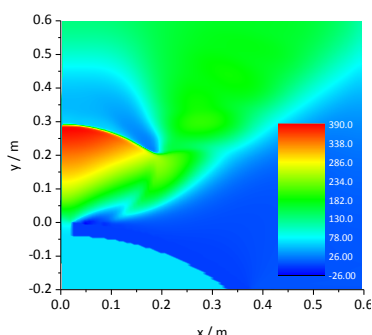

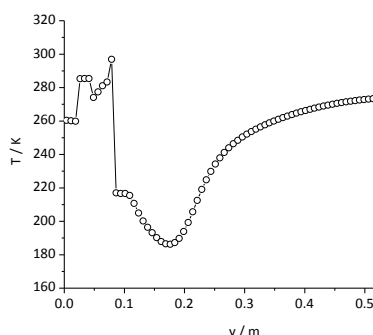Figure 6: Total velocity predictions at crack exit (m s^{-1})

Figure 7: Sample pipe-wall temperature predictions.

Figure 6 shows sample predictions of total velocity of a CO_2 release in the vicinity of the rupture outflow, as depicted in Figure 5. The structure of the under-expanded release clearly demonstrates associated phenomena such as the presence of stationary normal and oblique shocks. Figure 7 shows sample temperature predictions obtained from the calculation of a 0.2 m elliptical release in a 36 inch diameter pipe, observed along the centreline on the pipe-wall at x = 0. A significant drop in pipe-wall temperature is observed at the crack tip and the pipe is then exposed to further cooling with distance, due to being in contact with expanding fluid. A comprehensive numerical approach has been presented, that incorporates modelling strategies for interactions of supersonic multi-phase flow, complex thermodynamics, turbulence, and heat conduction.

References

1. Porter, R.T.J., Fairweather, M., Pourkashanian, M., and Woolley, R.M., *The Range and Level of Impurities in CO₂ Streams from Different Carbon Capture Sources.* **International Journal of Greenhouse Gas Control**, 2014. (accepted).
2. Woolley, R.M., Fairweather, M., Wareing, C.J., Falle, S.A.E.G., Proust, C., Hebrard, J., and Jamois, D., *Experimental Measurement and Reynolds-Averaged Navier-Stokes Modelling of the Near-Field Structure of Multi-phase CO₂ Jet Releases.* **International Journal of Greenhouse Gas Control**, 2013. 18(1): 139-149.
3. Donaldson, C.D. and Snedeker, R.S., *A Study of Free Jet Impingement. Part 1. Mean Properties of Free and Impinging Jets.* **Journal of Fluid Mechanics**, 1971. 45(2): 281-319.
4. Rotta, J., *Statistische Theorie nichthomogener Turbulenz. 1. Mitteilung.* **Zeitschrift fur Physik A-Hadrons and Nuclei**, 1951. 129: 547-572.
5. Khlifi, H. and Lili, T., *A Reynolds Stress Closure for Compressible Turbulent Flow.* **Journal of Applied Fluid Mechanics**, 2011. 4(2): 99-104.
6. Jones, W.P. and Launder, B.E., *The Prediction of Laminarization with a Two-Equation Model of Turbulence.* **International Journal of Heat and Mass Transfer**, 1972. 15(2): 301-314.
7. Gomez, C.A. and Girimaji, S.S., *Toward Second-moment Closure Modelling of Compressible Shear Flows.* **Journal of Fluid Mechanics**, 2013. 733: 325-369.

Predicting the atmospheric dispersion of carbon dioxide releases from pipelines for CCS applications using CO$_2$FOAM

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Abstract

This presentation reports on the development and validation of CO$_2$FOAM, a dedicated Computational Fluid Dynamics (CFD) solver for carbon dioxide (CO$_2$) dispersion, developed within the framework of the open source CFD code OpenFOAM® [1]. CO$_2$FOAM solves the three-dimensional conservation equations for a CO$_2$/air mixture for either the mean (ensemble-averaged) quantities or instantaneous quantities in a turbulent flow field. This involves solving the conservation equations of mass, momentum, energy and species concentration based on either the Reynolds-Averaged Navier–Stokes (RANS) approach or the Large Eddy Simulation (LES) approach. Energy conservation in the system is considered through the sensible-enthalpy equation. For consistency and numerical stability, the enthalpy of the mixture was assumed to be continuous when phase changes occur. In order to better capture the interaction between the dispersed CO$_2$ and the atmospheric specific boundary layer (ABL-specific), a compressible form of the k-ω Shear Stress Transport (SST) turbulence model is used in conjunction with ABL-specific wall-functions for turbulence modelling in the RANS approach. The Homogeneous Relaxation Model (HRM) approach is used to handle the presence of solid CO$_2$ within the release.

The code has been validated through experimental measurements in some full scale tests commissioned by National Grid within the dense phase CO$_2$ PipeLine TRANSportation (COOLTRANS) research programme [2,3]. Two approaches for handling the source conditions have been tested. The first approach uses the output from the near-field predictions generated by the University of Leeds to map out the input data for far field dispersion simulations while the second approach uses the pseudo source developed by DNV-GL on the basis of an existing model previously developed for natural gas pipelines and the new experimental data generated within COOLTRANS. Comparison of the predictions with experimental measurements in a puncture test will be presented. In the light of the difficulty for point to point comparisons of horizontal flows in a transient wind environment, a validation protocol involving the use of averaged data on each measurement arc has been tested and its merit will be discussed. The potential of using the pseudo source approach for the source condition modelling in simulating CO$_2$ dispersion from pipeline releases is highlighted while acknowledging that further comparison with independent data from other research programmes will be required to formulate a more conclusive recommendation.

Key words: Carbon dioxide, release from pipelines, CFD, Homogeneous Relaxation Model, validation with full scale data

References

1. http://www.OpenFOAM®.com.
2. Jennifer Wen, Ali Heidari, Baopeng Xu and Hongen Jie, Dispersion of carbon dioxide from vertical vent and horizontal releases—A numerical study, Proc IMechE Part E:J Process Mechanical Engineering, 227(2) 125−139, IMechE 2013.
3. Cooper R. National Grid's COOLTRANS research programme. J Pipeline Eng 2012; 11: 155−172.

IoLiCAP **CO$_2$QUEST**

A study of transient two-phase flows in CO$_2$ pipelines

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Abstract

For the transportation of the volume of CO$_2$ required by CCS to be economical the majority of CCS pipelines will need to be operated in the dense or supercritical-phase rather than in the vapour-phase [1, 2]. In Europe this will likely mean pipelines at line pressures above 100 bar passing through or near populated areas. Given that CO$_2$ is increasingly toxic at concentrations higher than 7% (v/v) the safety of CO2 pipelines is of great importance and indeed pivotal to the public acceptability of CCS as a viable means for tackling the impact of global warming.

Central to assessing the safety of such pipelines is the accurate prediction of the decompression and the discharge rate of the escaping inventory in the event of accidental pipeline rupture. Such data forms the basis for determining the minimum safe distances to populated areas, emergency response planning and the optimum spacing of emergency shutdown valves. In the case of a volatile fluid such as dense-phase or supercritical CO$_2$, by far the biggest challenge is the correct modelling of the ensuing complex flow dynamics associated with the transition from single to two-phase flow.

In the present study, performed as part of a UKCCSRC project [3], the development, testing and validation of a two-fluid transient flow model for simulating the outflow of CO$_2$ mixtures following pipeline failure is presented. Thermal and mechanical non-equilibrium effects during depressurisation are accounted for by utilising simple constitutive relations describing inter-phase mass, heat and momentum transfer in terms of relaxation directly to equilibrium. Pipe wall/fluid heat exchange on the other hand is modelled by coupling the fluid model with a finite difference transient heat conduction model.

The model's performance is tested by comparison of the predicted transient pressure and temperature profiles along the pipeline against those based on the simplified homogeneous equilibrium model (HEM) as well as real data captured during the full bore rupture of a 256m long, 233mm internal diameter pipeline (Figure 1) containing CO$_2$ at 36 bara and 273°C.

Figure 1. Photograph of an instrumented 256 m long, 233 mm i.d. pipeline for experimental studies of CO$_2$ releases.

The two-fluid model is found to produce reasonably good degree of agreement with the experimental data throughout the depressurisation process and, importantly, is found to capture the superheated

behaviour observed experimentally (Figure 2). The HEM based flow model on the other hand performs well only near the rupture plane and during the early stages of the depressurisation process.
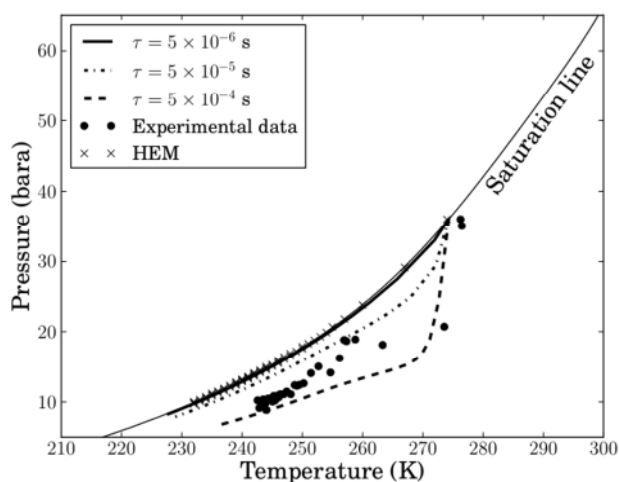

Figure 2. Thermodynamic trajectories measured and predicted following the initiation of decompression 10 m away from the rupture location [4]

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Measurement of Water Solubility Limits in CO_2 Mixtures to Ensure the Safe Pipeline Transportation of CO_2

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Abstract

Carbon Capture and Storage (CCS) is one of the more promising solutions to reduce CO_2 emission into the atmosphere.[1] There is an increasing literature on CCS, especially on CO_2 capture itself. Nevertheless, much work remains to be done before CCS is safe in the long-term. Particularly, the transport of CO_2 *via* pipelines from the power plant to underground reservoirs needs to be rigorously studied. Whatever the capture method (post-combustion, oxy-fuel or pre-combustion), the captured CO_2 will contain a small percentage of impurities including up to around 500 ppm of H_2O but also about 4% of other gases such as N_2, H_2 and Ar. Therefore, in order to prevent the rupture of the pipeline it is necessary to understand the effect of the impurities on the physico-chemical properties of the CO_2.[2, 3] Surprisingly, there are very few data to deliver water specification levels on CO_2 containing impurities mixtures.

In this context, our work has recently focused onto the solubility of water in CO_2 containing small percentages (5 and 10%) of N_2 at 313.15 K (40°C) in the pressure range 8 to 18MPa. These measurements have been carried out *in-situ* using an original high pressure-high temperature set-up coupled to an FT-IR spectrometer. Indeed, infrared spectroscopy allows an efficient quantitative study since water is very absorbing in the IR. Figure 1 shows that N_2 can lowered by up to 42% at 40°C the solubility of water in CO_2.
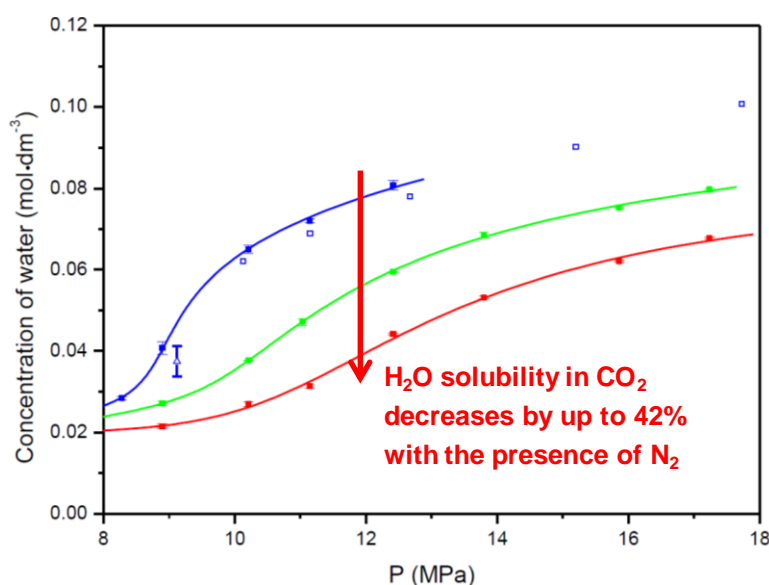
Figure 1. Evolution of the molar concentration of water: (■) in pure CO_2 from this work; (□) in pure CO_2 from King et al.1992; (△) in pure CO_2 from Wang et al. 2012; (■) in CO_2 + 5% N_2; (■) in CO_2 + 10% N_2 at 40 °C as a function of the pressure.

Further to this, we are currently developing a new independent and complementary method to reinforce our results since they represent important data for the safe transport of CO_2. This technique will also allow us to work under lower temperatures in order to be in appropriate conditions for Carbon Capture and Storage.

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IoLiCAP   **CO₂QUEST**

CO$_2$ Capture by Novel Supported Ionic Liquid Phase Materials Consisting of Silica Encapsulated Chitosan Ionogels

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Abstract

The urgent need for strategies to reduce global atmospheric concentration of greenhouse gases has prompted the development of novel efficient methods to capture CO$_2$ from flue gases. The conventional technology in industrial processes is currently chemical absorption of CO$_2$ with aqueous amines like monoethanolamine (MEA), diethanolamine (DEA) or methyldietanolamine (MDEA). However the method has several drawbacks like high energy input in regeneration step, additional operational cost due to degradation of amines, corrosion and environmental issues. Solid sorbents based on immobilized amines and amino-functional polymers like polyethyleneimine help to overcome these drawbacks and enable to achieve higher absorption capacities [1].

Sustainability, industrial ecology and green chemistry principles direct the development of next generation of materials and processes. Therefore chitosan, a natural amino-functional biopolymer, is proposed as an environmental friendly, renewable and inexpensive alternative for absorption of CO$_2$ [2]. The main problem related to applicability of biopolymers is their low solubility in common organic solvents due to strong inter- and intramolecular hydrogen bonds. Ionic liquids are known as powerful solvents for dissolving biopolymers. Furthermore ionic liquids also exhibit high CO$_2$ solubility. Due to specific properties like negligible vapour pressure, thermal stability and non-flammability ionic liquids have received interest as safe and easily recoverable CO$_2$ absorbents. Conventional ionic liquids absorb CO$_2$ through a physical absorption mechanism only. Therefore ionic liquids need to be combined with chemically active functional groups or materials to obtain higher absorption capacities [1].

In the current research a novel sorbent for capture of CO$_2$ was developed by combining chemical absorption by chitosan and physical absorption by ionic liquids. Different commercial and custom made ionic liquids were investigated for solubilisation of chitosan. Up to 10% chitosan can be dissolved in ionic liquids depending on the hydrogen bong acceptor properties of anion. Obtained chitosan ionogels were immobilized using a solid silica support to increase specific surface area and thereby achieve higher CO$_2$ absorption capacities. Based on the idea of "dry water" and "dry ionic liquids" [3] new inverse SILP (supported ionic liquid phase) systems were developed. In common SILP systems an ionic liquid layer is formed on the porous support material but in inverse SILP on the contrary ionic liquid droplets are covered with fumed silica particles [4]. CO$_2$ absorption capacities of the prepared materials were measured and will be presented.

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Optimised PEI impregnation of activated carbons - Enhancement of post-combustion CO_2 capture

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Abstract

A virgin activated carbon (denoted as AR) was successfully modified through Polyethylenimine (PEI) impregnation, which was carried out according to the procedure reported by Xu [1]. Virgin and PEI-impregnated samples were tested for CO_2 capture under post-combustion conditions (53 °C, 15 % CO_2/85 % N_2) by using a thermogravimetric analyser (TGA). Unlike previous studies [2], in addition to the influence of PEI loading, the effect of the stirring time of the mixture PEI/methanol/carbon onto the CO_2 sorption capacity of the modified carbons was also assessed. In particular, it was found that a longer agitation entailed attaining higher uptakes, likely due to a better dispersion of the polymer onto the support's pores. N_2 adsorption measurements revealed a reduction of surface areas and pore volumes due to the polymer impregnation onto the carbons' pores. Nevertheless, all the modified samples exhibited larger uptakes than the virgin carbon's, which CO_2 capacity was increased up to four folds. This outstanding enhancement was attributed to the N-based functionalities incorporated onto pristine carbon's surface after the PEI impregnation. These were detected by XPS analyses, which confirmed the effectiveness of the surface modification. This result is corroborated by the increased N content measured for PEI-modified samples by elemental analysis (CHNS). Amino groups ensured a higher selectivity of the sorbents toward carbon dioxide molecule. Furthermore, optimal PEI-impregnated carbon (i.e. AR_PEI_60 _4h) showed larger uptakes and faster kinetics than those attained by Z13X (commercial zeolite) included for comparison purposes. These findings indicated that optimised PEI impregnation was an effective route to enhance the post-combustion capture performances of activated carbons.

Sample ID	TGA 15% CO_2, 53 °C (mgCO_2/g$_{sorb}$[1])	N_2 adsorption isotherms S_{BET}[2] (m^2/g)	V_{mi}[3] (cm^3/g)	CHNS N (wt. %)
AR[4]	8.3	1531	0.569	0.37
AR_PEI_40 _1h	24.0	933	0.346	4.87
AR_PEI_60 _1h	23.0	893	0.330	4.91
AR_PEI_60 _4h[5]	33.7	880	0.331	6.71
AR_PEI_80 _1h	28.3	943	0.355	5.53
AR_PEI_100 _1h	26.9	936	0.349	5.88
Z13X[6]	30.7	543	0.207	0.00

Table 1. Post-combustion CO_2 uptakes, textural parameters and nitrogen content for virgin and PEI-impregnated carbon carbons.

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[1] Sorb stands for sorbent
[2] BET surface area
[3] Microporous volume
[4] Virgin carbon
[5] PEI impregnated carbon; PEI/AR ratio = 60 wt. %; solvent = Methanol
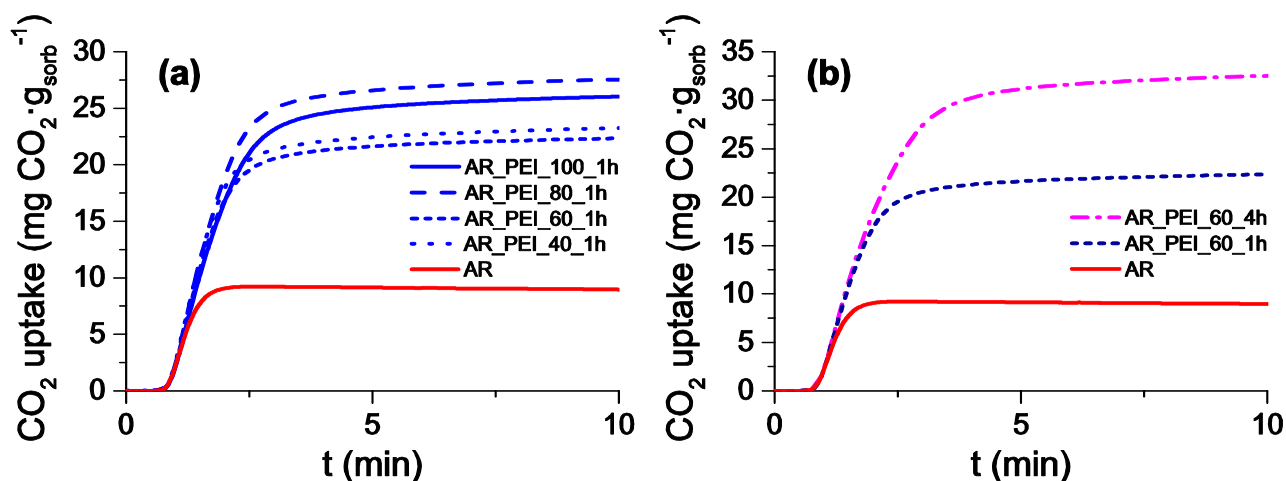[6] Commercial zeolite

Figure 1. CO_2 uptakes under post combustion conditions (15% CO_2 and 53 °C) for virgin and modified carbons: Effect of PEI loading (a) and stirring time (b).
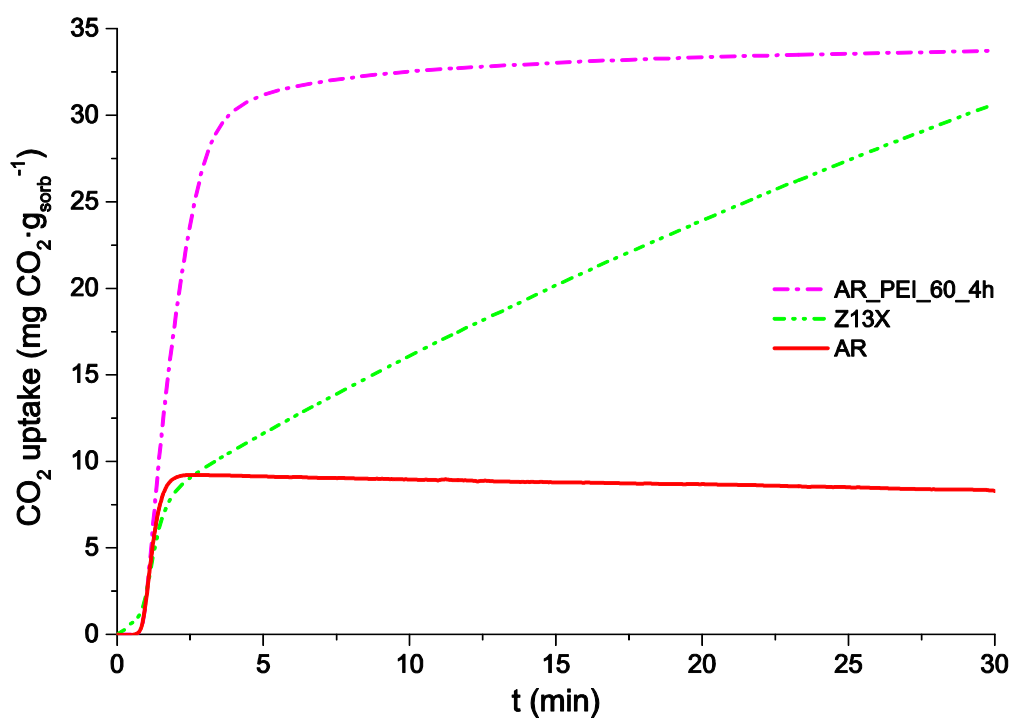

Figure 2. CO_2 uptakes under post combustion conditions (15% CO_2 and 53 °C): Comparison between optimal PEI-impregnated carbon and Z13X

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Molecular Simulation of Ionic Liquid Solvents for CO$_2$ Capture

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Abstract

Ionic liquids (ILs) are organic salts with melting points usually near room temperature (RTILs). ILs exhibit a unique combination of properties such as extremely low vapor pressures, thermal stability, chemical tunability, good electrolytic and solvation properties, non-flammability and easy recycling. These properties are also combined in many cases with a remarkable CO$_2$ absorption capacity and selectivity [1] that renders ILs among the most promising solvents for CO$_2$ capture and separation from post-combustion flue gases [2], fulfilling at the same time many environmental aspects of the post combustion CO$_2$ capture (PCC) technology. The chemical diversity in the molecular structure of the ions involved affects directly the physicochemical properties of the ILs, thus enabling the tuning of the properties of an IL by making moderate changes in ions' chemical formula and structure. Molecular simulation methods are proven to be extremely valuable in the direction of screening the most promising systems by reliable property prediction strategies as well as by revealing a wealth the microscopic information [3,4] on the underlying mechanisms that are responsible for the macroscopic behaviour of ILs aiming at the design of solvents with tailor-made properties.

The present work focuses on the molecular simulation of imidazolium-based [TCM-] ionic liquids using an optimized classical atomistic force field. Long molecular dynamics (MD) simulations of the [C$_n$mim$^+$][TCM$^-$] ILs family have been performed at various temperatures and at atmospheric pressure in order to calculate the thermodynamic, structural and transport (self-diffusion coefficients and viscosities) properties of the pure ILs, exploring, simultaneously, the intrinsic characteristics and mechanisms of the systems under study at the atomistic level. Additional very long MD simulations were performed for the calculation of gas (CO$_2$, N$_2$, CH$_4$, Ar and O$_2$) diffusion coefficients that were estimated one order of magnitude less than the ions' self-diffusivities while all gases appeared to have comparable diffusivities, in agreement to experimental measurements. Gas solubilities were calculated in the Henry's law regime using the Widom test particle insertion method, with the solubility of CO$_2$ being much higher than the one of the other gases. The influence of the temperature and the cation's alkyl chain length on the above mentioned properties was thoroughly investigated as well as the effect of confinement in the structure and dynamics of these ILs.

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IoLiCAP   **CO$_2$QUEST**

Comparative costings for 1st, 2nd and 3rd Generation CCS Technologies

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Abstract

Drawing on both the literature and current research projects, the cost of CCS will be assessed for technologies likely to be applied in the short, medium (5 – 10 yrs) and long (10 + years) terms. A particular focus will be high temperature solid looping cycles, which are a relative newcomer in the field of CCS, but are being rapidly commercialised.

The economics of any process are key to its uptake. It is important to remember this when considering CCS technologies, which are marginally incentivised in the EU, but will eventually be crucial to efforts to combat climate change. As regulation of CO2 emissions becomes more stringent, operators have renewed focus on the bottom line, driving renewed interest in 2nd and 3rd generation technologies. This study will mainly use the cost of CO2 avoided as its primary metric. A significant number of literature sources have yielded costs, which have then been re-based to 2011 USD for fair comparison.

A very approximate price for Ca-looping is estimated to be **$\$_{2011}26 \pm 10$**, with chemical looping yielding costs in the region of **$\$_{2011}20 - 30$** for application to a power station. Costs for a variety of industrial sources of CO¬2 have also been surveyed; these have been found for the iron and steel **($\$_{2011}55 - 85$)**, refining **($\$_{2011}60 - 95$)**, pulp and paper **($\$_{2011}39 - 60$)** and cement industries **($\$_{2011}38 - 122$** with a clear split in costs between MEA scrubbing and oxyfuel or Chemical Looping Combustion).

A key message is that it is extremely important to consider how the financing has been accounted for in any analysis, prior to quoting a figure.

Computationally efficient surrogate based multi-objective optimisation for pressure swing adsorption for Carbon capture

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Abstract

Pressure swing adsorption (PSA) processes have the potential to achieve higher productivity compared with alternative separation processes and are particularly relevant for post-combustion carbon capture in coal or gas fired power plants. The design of integrated carbon capture, however, requires the dynamic modelling of the process behaviour. This leads to large computational requirements and typically makes an optimisation based design approach intractable.

Traditionally, the computational challenge is addressed through the use of simpler models. However, these models may not capture the detail required to identify the best designs, especially in a multi-objective scenario where potentially conflicting criteria are used to evaluate and compare alternative designs. This paper presents a *surrogate based optimisation* (SBO) procedure which addresses the computational challenge through the automatic and adaptive definition of surrogate models. The surrogate model is introduced into an optimisation procedure as illustrated in Figure 1; the full model is used periodic update and validation.

The NSGA-II method [2] has been used extensively for multi-criteria design problems. It is a genetic algorithm suitable for optimisation where gradient information is not present and where the convexity of the objective function, the constraints and even the design space is not an issue. The method provides a number of features which are necessary for design, including diversity control for ensuring the Pareto trade-off curve approximated is as broad as possible and is able to incorporate design points which are infeasible into the selection procedures. We have used NSGA-II as the basis for our SBO.

Two implementations have been developed, one using the NSGA-II along with a kriging based surrogate model [1] and one which introduces Active Learning MacKay (ALM) [4] to broaden the approximation to the Pareto front. The implementations make full use of parallel computing and has been tested on an 8 core system, yielding close to linear speed-up.

A case study for the separation of a flue gas with composition 15% CO_2 and 85% N_2 has been investigated. For this case study, a two column six step PSA system is considered, simulated using the CySim General Adsorption Cycle Simulator [3]. There are 6 design variables: purge to feed ratio, feed/purge time, feed flow rate, vacuum pressure, valve stem positions and feed temperature. With simulation times ranging from minutes to hours for a single design point, the problem has been attempted with a constraint on the number of objective function evaluations. The results, comparing the two approaches described above and the NSGA-II procedure using the detailed model directly, are presented in
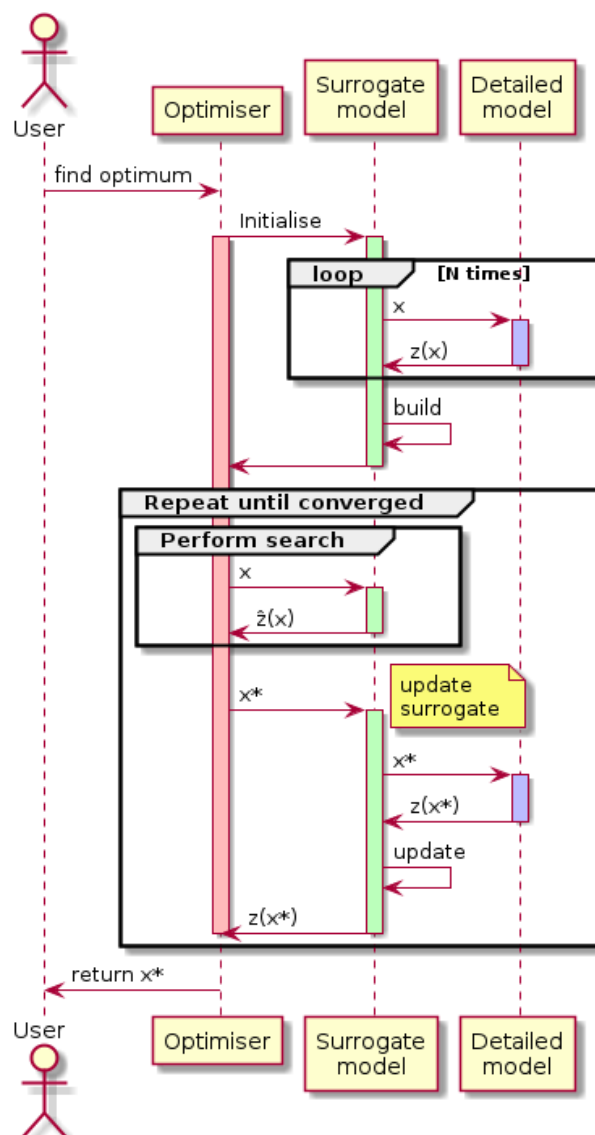
Figure 1. Sequence of operations for surrogate based optimiser showing use of detailed and surrogate models.

terms of the final populations, shown in Figure 2. The surrogate based methods are able to find designs that achieve high values of both purity and recovery. Without the surrogate, no good solutions are found within the computational constraints.
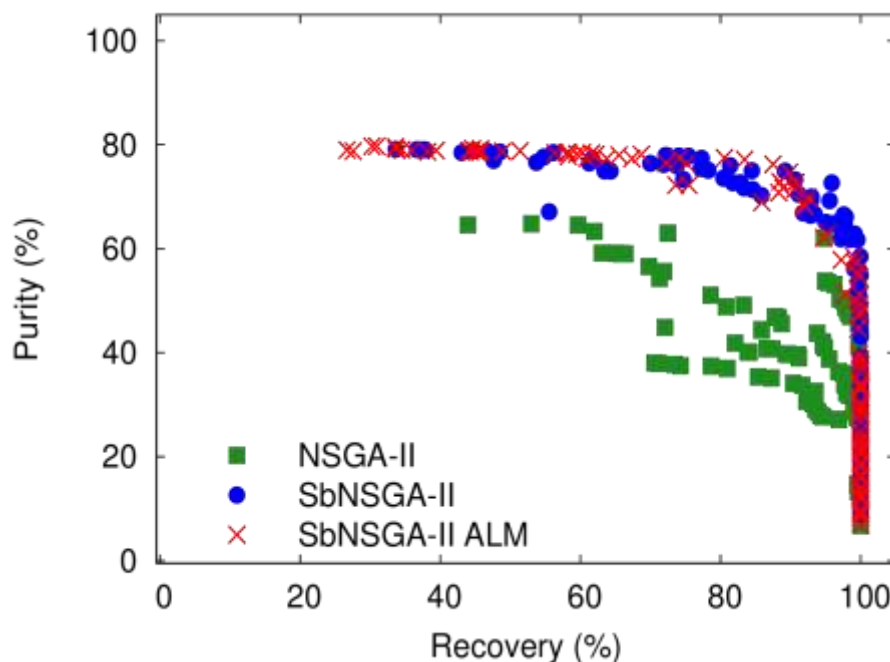

Figure 2. Final populations obtained with 256 detailed function evaluations for each method, showing the significantly better approximation to the Pareto front obtained with both SBO methods.

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IMPACTS: Economic Trade-offs in
Establishing CO$_2$ Impurity Specifications

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Abstract

The IMPACTS project has a stated broad objective to develop the knowledge base of CO$_2$ quality required for establishing norms and regulations to ensure safe and reliable design, construction and operation of CO$_2$ pipelines and injection equipment, and safe long-term geological storage of CO$_2$.

The relationship between CO$_2$ quality and CCS system design and performance is relevant, not only for single source – single sink project, typical for demonstration projects, but also for more complex, multi-user systems or networks. A sound knowledge base is required concerning the complex impact of CO$_2$ quality on fluid properties and materials and, hence, its influence on the transport and storage system.

More specifically, the focus for this paper is how the project sets out to reveal the impacts of relevant impurities in the CO$_2$ stream on the design, operation and costs of the capture, transport and storage infrastructure so as to provide recommendations for optimized CO$_2$ quality through techno-economic assessments (amongst other considerations). This paper gives an overview of the work being carried in various areas including fundamental properties, corrosion, and the injection and storage processes and reports on the derivation of the influences of CO$_2$ quality on these aspects. These influences are combined with modelling of the cost of measures to mitigate or prevent them from affecting the operation of the CCS system, or of adapting the CCS system design. Thus, the impacts can be set out as a set of cost functions relating to capex and opex and including the effects overall availability, process efficiency changes and health and safety overlays. A specifically designed CCS chain model is used to assess the impacts on a number of representative benchmark CCS chains, carrying out comparative economic trade-offs to both understand the full-chain whole-life economics of certain CO$_2$ impurities at different levels and then to potentially propose optimized purity specifications for various sets of circumstances.

The paper will update and extend previous reporting of progress in the IMPACTS project, such as Eickhoff et al. [1]. It is intended to be complementary to a paper submitted to the same forum by Professor R Span of Bochum University which will cover more fundamental work in IMPACTS on properties of CO$_2$ impurities.

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IoLiCAP   CO$_2$QUEST

Techno-economic analysis of gas purification for CO$_2$ transport and injection for storage

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Abstract

As Carbon Capture and Storage (CCS) is coming closer to its commercial deployment in the UK – with the Peterhead and White Rose CCS projects – and in the EU – with the Rotterdam Capture and Storage Project (ROAD) – it is crucial to optimise every step of the process and understand how each step is linked; from capturing the CO$_2$, to its subsequent purification, transport, injection, and finally, sequestration. Oxy-fuel power plants, currently one of the most promising CCS technologies, produce one of the least pure streams of CO$_2$ (Posch et al. (1)). Therefore, an additional gas purification unit needs to be added to the capture plant prior to its transport and storage. As part of the DYNAMIS project (de Visser et al. (2)) a set of CO$_2$ stream purity recommendations were presented, specifying the required purity of a given CO$_2$ stream as a function of the injection sink (see Table 1). For example, a 100-1000ppm limit on O$_2$ content is recommended for use in enhanced oil recovery (EOR) whereas for storage in saline aquifers O$_2$ should be less than 4vol%. The strict limit on O$_2$ levels in CO$_2$ streams for EOR stems from a set of risks triggered by the presence of O$_2$ in oil reservoirs. These include overheating at the injection point and biological growth (Pipitone et al. (3)). The recommendations also include limits on water content owing to the effect it can have on pipeline corrosion, limits on the amount of non-condensable gases due to the added compression work their presence requires and their impact on minimum miscibility pressure (MMP) affecting CO$_2$-EOR, and limits on the level of toxic components such as H$_2$S due to health and safety concerns. These aim to maximise health and safety and operation and design. A study conducted by Yan et al. (3) concurs with the recommendations given by the DYNAMIS project regarding the maximum amount of non-condensable gases, although they note that 10vol% is acceptable for transport over short distances. However, in the context of these recommendations, there has been very little focus on connecting this purification step with the other CCS steps, and there is, thus far, no general or international consensus on the purity requirements for CO$_2$ transport via pipelines (Boot-Handford et al. (4)).

	a. Flue gas composition range (by volume) from coal-fired oxy-combustion plants (1)	b. Weyburn EOR project CO$_2$ composition by volume (7)	c. Sheep Mountain Reservoir typical CO$_2$ composition by volume (8)	d. Dynamis recommendations for CO$_2$ quality by volume (1)
CO$_2$	72.4% - 76.4%	>96%	97%	>95.5%
C$_x$H$_y$	0	<0.7%	2.4%	<4% (saline aquifers) <2% (EOR)
CO	0	<1000ppm	-	<2000ppm
H$_2$S	0	<9000 ppmv	-	<200 ppm
N$_2$	11.3% - 14.2%	<300ppm	0.6%	<4%
O$_2$	7.8% - 9.5%	<50 ppm	-	<4% (saline aquifers) 100-1000ppm (EOR)
Ar	2.8% - 3.11%	-	-	<4%
SO$_2$	~0.01%	-	-	<100ppm
SO$_3$	0	-	-	-
NO	0	-	-	<100 ppm
H$_2$O	1.0% - 1.4%	<20 ppm	trace	<500 ppm

Table 1.   Typical oxy-combustion flue gas composition (a.), typical CO$_2$-EOR gas compositions (b. & c.) and CO$_2$ stream quality recommendations (d.)

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In this work, a CO_2 compression and purification unit from a pulverised fuel oxy-combustion plant is modelled in Aspen HYSYS. This model builds on similar separation processes presented by Posch et al. (1) and Pipitone et al. (5). From the model, results are obtained for different levels of separation efficiency and different impurity content. This includes the added compression work and cooling duty required for incremental purity or recovery, and the effect this has on the plant's operational and capital costs. A change in capital costs can include the addition or elimination of a compressor, a cooler or a flash unit. A quantitative relationship is established between the cost of increased purification and the purity of the CO_2 stream and a cost-benefit analysis for high-purity CO_2 and low purity CO_2 is performed. In the context of CO_2-EOR, the cost-benefit analysis is highly dependent on the price of oil. As EOR is one of the major economic incentives for the deployment of CCS (Kuuskraa et al. (6)), this paper focuses on meeting the requirements for a CO_2-EOR applicable stream.

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CCS System Modelling: Enabling Technology to Help Accelerate Commercialisation and Reduce Technology Risk – A Case Study on the Operation of CCS Networks

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Abstract

The commercial implementation of CCS still faces significant challenges. Many of these arise from the fact that the whole chain and, eventually, whole CO2 transportation network needs to be considered as a single system in order to make design and operation decisions that satisfactorily address the commercial imperatives and risk requirements of the various stakeholders along the chain. Even a quick analysis shows that design and operating decisions at the power plant can have a significant effect on storage providers at the other end of the chain, and vice versa. A systems modelling approach is essential, but there are currently no tools that can satisfactorily provide this capability over the whole CCS chain.

In order to address this, a £3m project was commissioned and co-funded by the ETI and project participants, who comprise E.ON, EDF, Rolls-Royce, CO2DeepStore, Process Systems Enterprise (PSE) and E4tech. The project is aimed at delivering a robust, fully integrated tool-kit that can be used by CCS stakeholders across the whole CCS chain. This tool-kit will be released as a commercially-supported software product at the end of the project.

This presentation describes the results of a case study for a CCS network comprising capture from a supercritical pulverised-coal (located in Grangemouth, Scotland) and a combined-cycle gas turbine (located in Peterhead, Scotland) power plant, two compression stations and transport to injection in two subsea formations for storage (Goldeneye and Captain Clean) both located at the Captain Sandstone Aquifer. Figure 1 illustrates the representation in gCCS [1] of the overall CCS network in study.
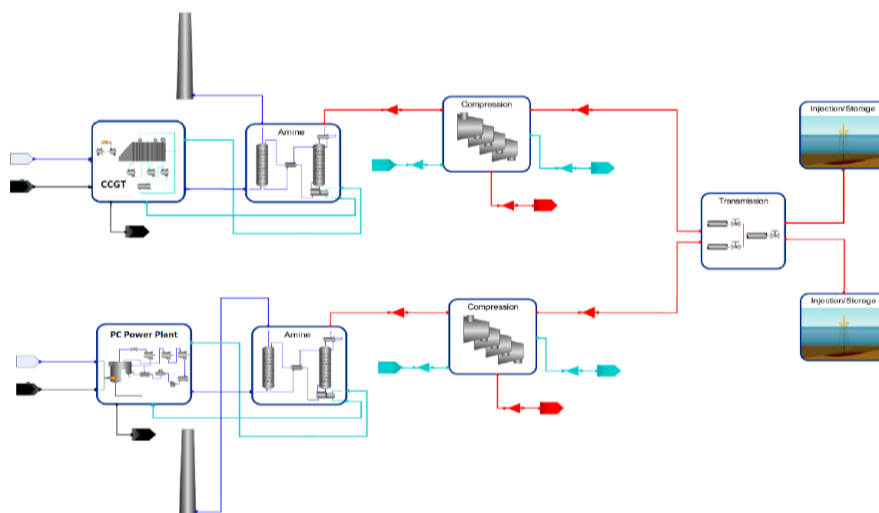
Figure 1. High-level representation of the overall CCS network

Several steady-state scenarios were considered and results were obtained for different power plant loads, CO2 capture rates and phases in the transportation network (both gas and dense phase were studied). In an electricity network, a Pulverized Coal Power Plant (PCPP) usually corresponds to a base load power plant, while a Combined Cycle Gas Turbine (CCGT) plant is more likely to be a load following power plant. Therefore, it has been decided to keep the PCPP load always equal to, or greater than, the CCGT load in the different scenarios. The aim of the variable load

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scenarios is to analyse the impact of reduced power plant loads on the downstream sub-systems of the CCS chain during steady operation.

Dynamic scenarios include load variation of one of the power islands for both gas phase and dense phase of CO2 transportation and emergency shut-down slam shut of pipeline.

The load variation dynamic scenario corresponds to a ramp-up/ramp-down cycle for the CCGT will represent a case of peak load demand and its consequences for the CO2 network. This scenario was performance for two different pressures at the reservoirs in order to have different phase of the CO2 transported in the pipeline network (one at the gas phase and another run at dense phase). The objective is to compare both scenarios and understand the impact of the phase of the transported CO2 in both performance but also operability of the all chain during transient events like peak load.

Some key results of the load variation scenario are illustrated in Figure 2:
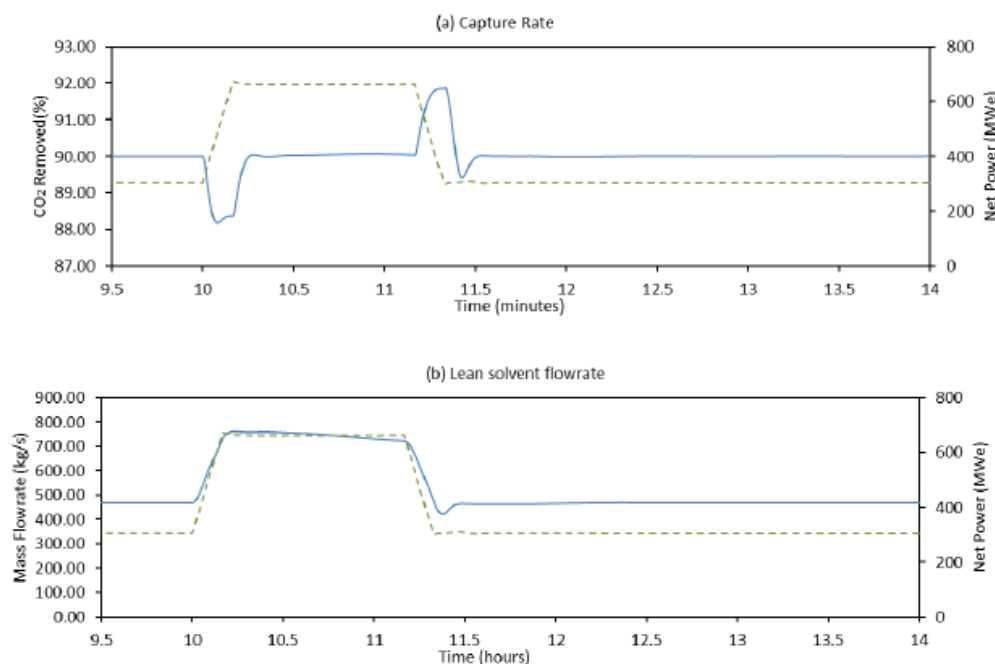
Figure 2.Response of capture plant variables (a) Rate of absorbed CO2 (b) Lean solvent flowrate to the absorber. The dashed green lines represent the variation of net power, while the continuous blue lines represent the other values

The Emergency Shut-down slam shut scenario considers the effect of an emergency closure (a "slam shut") of the onshore Emergency Shutdown (ESD) valve. The objective of this scenario is to evaluate the effect on the transmission network of an ESD valve, specifically considering the impact of a "slam shut" in the pipeline, evaluating and reporting any short term transients observed in the pipeline and its impact on the power stations, evaluating how quickly the compression stations need to stop pumping CO2 into the pipeline.

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Thermophysical Properties of Tricyanomethanide- and Tetracyanoborate-Based Ionic Liquids by Using Dynamic Light Scattering and Conventional Methods

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Abstract

In the present study, thermophysical properties of ten low-viscosity ionic liquids (ILs) based on the anions $[C(CN)_3]^-$ (tricyanomethanide) and $[B(CN)_4]^-$ (tetracyanoborate) and carrying a homologous series of [alkyl-MIM]$^+$ (1-alkyl-3-methylimidazolium) cations [EMIM]$^+$ (ethyl), [BMIM]$^+$ (butyl), [HMIM]$^+$ (hexyl), [OMIM]$^+$ (octyl), and [DMIM]$^+$ (decyl) were investigated by using conventional methods and dynamic light scattering (DLS). For these ILs currently discussed regarding their potential use in carbon dioxide separation processes or solar cell applications, an Abbe refractometer was used for the measurement of the refractive index in the temperature range from (283.15 to 313.15) K at atmospheric pressure with an expanded uncertainty ($k = 2$) of 0.0005. The density was measured between (283.15 and 363.15) K at atmospheric pressure with a vibrating-tube densimeter and an expanded uncertainty ($k = 2$) of 0.02%. The thermal conductivity was obtained by a steady-state guarded parallel-plate instrument between (283.15 and 353.15) K at atmospheric pressure with an expanded uncertainty ($k = 2$) of 5%. The corresponding results were used for the development of an improved prediction scheme for the thermal conductivity of arbitrary ILs. For the cation and in case of the $[B(CN)_4]^-$-based ILs also for the anion, the self-diffusion coefficients were obtained from nuclear magnetic resonance (NMR) spectroscopy from (273.15 to 318.15) K at atmospheric pressure with an expanded uncertainty ($k = 2$) of 10%. The interfacial tension was measured with the pendant-drop technique at about 295 K and atmospheric pressure with an expanded uncertainty ($k = 2$) of 1%. Based on this datum and the temperature dependence of the density, the interfacial tension for all relevant temperatures was estimated via an appropriate prediction model. For the optically transparent $[B(CN)_4]^-$-based ILs, the ratio of dynamic viscosity to interfacial tension could be directly accessed by surface light scattering (SLS) in a first order approximation. Combining the results from SLS with those for density and interfacial tension from conventional methods, the dynamic viscosity could be obtained in the temperature range from (283.15 to 363.15) K at atmospheric pressure with an expanded uncertainty ($k = 2$) of less than 3%. For measuring the viscosity of semi-transparent liquids such as the $[C(CN)_3]^-$-based ILs by using DLS, light scattering from dispersed particles was tested as further possible measurement technique. For four $[C(CN)_3]^-$- and $[B(CN)_4]^-$-based ILs forming stable particle dispersions, the dynamic viscosity was obtained in a temperature range between (283.15 and 353.15) K at atmospheric pressure with an expanded uncertainty of less than 5% ($k = 2$). For binary mixtures of [BMIM][C(CN)$_3$] and [BMIM][B(CN)$_4$] with dissolved carbon dioxide, DLS from the bulk of fluids was applied for the measurement of the mutual diffusivity at macroscopic thermodynamic equilibrium. The data were obtained at temperatures between (303.15 and 333.15) K and pressures between (2 and 26) bar and have a typical expanded uncertainty ($k = 2$) of less than 10%. All results were compared with literature data and show the influence of the varying alkyl chain length in the cation as well as of the different cyano-based anions on the thermophysical properties of the studied IL systems.

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Solubility and Kinetics of CO_2 in Low Transition Temperature Mixtures: Experiments and Modeling

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Abstract

The growing level of CO_2 emissions from industrial fixed-point sources is one of the most pressing environmental concerns of our time. Carbon Capture and Storage (CCS) are considered as a promising route to reduce the CO_2 emissions in the near-term. Carbon capture accounts for about 80% of the overall costs of the CCS process. Capturing and compressing CO_2 increase the fuel needs of a coal-fired CCS plant by 25-40%. Selexol (a mixture of dimethyl ethers of polyethylene glycol) is often utilized as solvent in the pre-combustion configuration. However, refrigeration required to lean the solvent and the co-absorption of hydrocarbons make this process less efficient. Hence, this section of the CCS deserves additional attention where improvements will have the highest effect on cost reduction

The potential of a new type of solvents, so-called low transition temperature mixtures (LTTMs) or deep eutectic solvents (DESs), as sustainable substituents for the conventional CO_2 absorbents is explored. LTTMs are mixtures of two solid compounds, a hydrogen bond donor (HBD) and a hydrogen bond acceptor (HBA), which form liquids upon mixing with melting points far below that of the individual compounds. In this work the HBD is lactic acid and the HBAs are tetramethylammonium chloride, tetraethylammonium chloride and tetrabutylammonium chloride. Although their physicochemical properties are similar to those of ionic liquids (ILs), LTTMs are much cheaper, easy to prepare, biodegradable, tunable (nature of the HBD and HBA and their ratio can be chosen) and less toxic, hence avoiding complex purification steps and large waste disposal encountered with ILs.

The thermal operating window (e.g., glass transition and decomposition temperature) and physicochemical properties (e.g., density, viscosity and surface tension) of several novel developed LTTMs for CO_2 capture have been determined. A thermogravimetric technique based on a magnetic suspension balance operating in static mode was applied to study the thermodynamics (i.e., absorptive capacity and Henry's law coefficient) and kinetics (i.e., diffusion coefficient) at several temperatures and pressures up to 20 bars. The influence of LTTM composition and water content on the CO_2 solubilities and diffusivities was established. It will be shown at the conference that LTTMs are promising sorbents for pre-combustion CO_2 capture due to their high capacity (at high pressures) and their low regeneration energy consumption (low heat of absorption).

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Measurements on Volumetric Properties of binaries and ternaries of Carbon dioxide, Nitrogen, and Argon at Supercritical State by Single Sinker Densimeter

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Abstract

A single sinker densimeter was built to fill the gap of volumetric knowledge of fluids for carbon capture and storage. The densimeter was manufactured by Rubotherm GmbH, Germany and specially designed for measuring gas or supercritical fluids with corrosion resistivity in the following range: $273.15 \leq T/\text{K} \leq 423.15$, $0 \leq p/\text{MPa} \leq 35$. The measuring system is schematically illustrated in Figure 1.
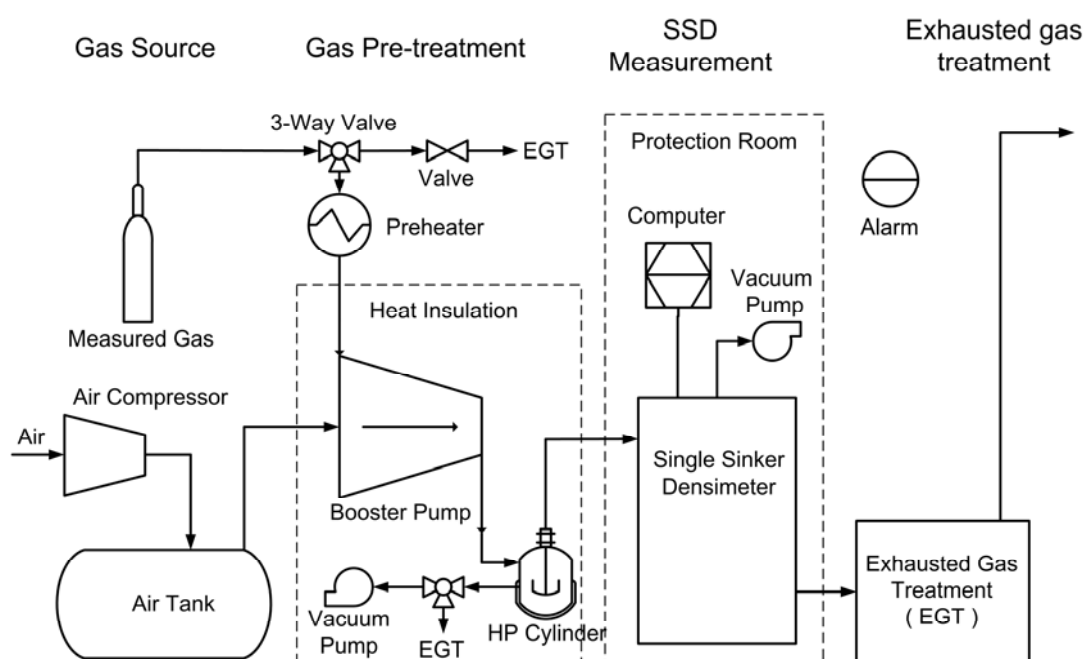
Figure 1 Density measuring system

The extended uncertainties ($k=2$) of the densimeter are 35.1 mK for temperature, 3.39 kPa for pressure, and 0.026% for density, respectively. The combined density measurement uncertainty ($k=2$) is from 0.043% at 11 MPa to 0.031% at 31 MPa on purity. Measurement results on pure N_2, Ar, and CO_2 are within measurement uncertainty, but have similar systematic deviation from state-of-the-art equations of state (N_2 [1], Ar [2], CO_2 [3]). This systematic deviation was partially compensated by a correction function built merely based on N_2 measurement. The correction function is fluid independent as least among N_2, Ar, CO_2, and their mixtures.

Mixtures ($0.05\ CO_2 + 0.95\ N_2$), ($0.01\ CO_2 + 0.99\ N_2$), ($0.05\ CO_2 + 0.95\ Ar$), ($0.01\ CO_2 + 0.99\ Ar$), ($0.90\ CO_2 + 0.05\ N_2 + 0.05\ Ar$), ($0.95\ CO_2 + 0.04\ N_2 + 0.01\ Ar$) at 298.15 K to 423.15 K and 11 MPa to 31 MPa were measured. Volumetric properties of these mixtures have not seen in literature before. The composition uncertainty was declared to be within molar 0.1% ($k=2$) by the gas provider and the contribution to density uncertainty from absorption and desorption effects could be as high as 0.1% [4]. Therefore, the combined density measurement uncertainties ($k=2$) are 0.15% on

CO_2–N_2, 0.12% on CO_2–Ar, and 0.45% on CO_2–N_2–Ar. Uncertainty in composition is the dominative uncertainty in mixture measurements, yet it is estimated exceedingly conservatively.

   Examples of measurement results are shown in Figure 2. Generally they are within uncertainty of GERG-2004 EOS [5]. The experiment results could be used to further improve the performance of multi-parameter equation of state models for mixtures. The research leading to these results has received funding from the European Community's Seventh Framework Programme (FP7-ENERGY-20121-1-2STAGE) under grant agreement n°308809 (The IMPACTS project).
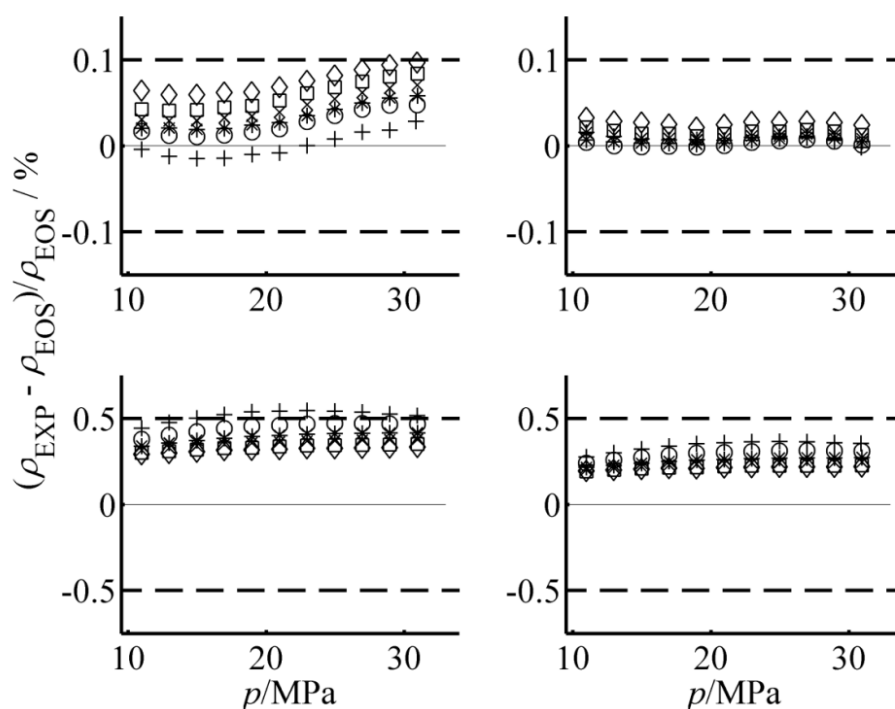

Figure 2 Relative deviations from experiment results to GERG-2004 EOS [5] at temperatures from 298.15 K to 423.15 K and pressures from 11 MPa to 31 MPa on 0.05 CO_2 + 0.95 N_2 (up left), 0.01 CO_2 + 0.99 N_2 (up right), 0.05 CO_2 + 0.95 Ar (down left), and 0.01 CO_2 + 0.99 Ar (down right). Dashed lines are uncertainty boundaries of GERG-2004 EOS.
+ 25 °C; ○ 50°C; * 75°C; × 100°C; □ 125°C; ◇ 150°C.

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Thermophysical Properties for Transport and Storage of CO_2-rich Mixtures – Contributions by IMPACTS

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Abstract

In 4 subprojects and 13 work packages, the FP 7 project "Impact of the Quality of CO_2 on Transport and Storage", IMPACTS, addresses issues related to transport and storage of CO_2-rich mixtures resulting from carbon capture and storage applications. The project focusses on the impact of impurities in the CO_2 on safety and commercial viability of transport and storage scenarios. For this reason fluid-dynamic, corrosion and thermophysical-property effects on safety, material and site selection, and finally economy are considered. The goal is to develop a "tool box" enhancing our ability to develop an optimum design for transport and storage equipment.

In this context, WP1.2 of IMPACTS addresses an improved description of thermophysical properties of CO_2-rich mixtures. Experimental work is carried out at Ruhr-University Bochum and at Tsinghua University. Both universities measure densities of relevant binary and multicomponent systems containing CO_2 and / or the components expected as most relevant impurities. Ruhr-University additionally addresses dew points of mixtures with a relative permittivity apparatus. In the second implementation phase, SINTEF will join the experimentally working team with its newly developed phase-equilibrium equipment.

On the theoretical side available models for thermodynamic and transport properties were evaluated. This process resulted in practical recommendations for models, which represent the "state of the art". With regard to thermodynamic property models, the work within IMPACTS contributes to a broader approach at Ruhr-University. For many applications the GERG 2004/2008[1], which was originally developed to describe properties of natural gases, proved to be an appropriate property model. Shortcomings of the GERG 2004/2008 model were found particularly for the system CO_2/H_2O, which is essential for many processes in carbon capture and storage. Improved mixing models for this and other relevant subsystems have been developed[2]; experimental campaigns aiming at an improved data base for mixtures relevant for carbon capture and storage are on their way.

The focus of theoretical work is currently shifting towards an accurate description of the complex phase equilibria relevant for carbon capture and storage, which is supposed to be consistent to the results of reference models in the single-phase regions. The adapted reference model for the fluid phase accurately describes vapour/liquid equilibria as well as liquid/liquid equilibria. It has been shown that not only ice and dry ice, but also the formation of hydrates[3] can be described consistently to an accurate description of the fluid phases with new models.

The presentation will give an overview of the thermophysical-property activities in IMPACTS. The status of the development of property models at Ruhr-University will be discussed in more detail.

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Prediction of Physical Properties for CCS Process Design Using Molecular Simulation

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Abstract

Accurate knowledge of thermodynamic and transport properties and phase equilibria of CO_2 mixtures over a wide range of temperature and pressure is critical for the optimum design of CCS processes. These properties can be either measured experimentally or calculated using appropriate models. Experimental measurements are time consuming and costly. Thermodynamic models in the form of equations of state, activity coefficient models or simple empirical correlations are used widely for process design calculations. In this case, some experimental data are needed to tune interaction parameters of the models. A powerful approach evolved in recent years refers to molecular simulation. Thanks to the unprecedented increase of computing power and the development of accurate atomistic force fields, molecular simulation can be used to generate reliable predictions for various physical properties of complex chemical systems, in the absence of experimental data.

In this work, various two-body atomistic force fields for H_2O, CO_2 and NaCl were used to calculate a spectrum of properties. In all cases, extensive comparison against experimental data was performed. Gibbs Ensemble Monte Carlo (GEMC) simulations were used to predict H_2O – CO_2 phase equilibria from 423 K to 523 K in the pressure range 200 – 800 bar [1]. It was found that an exponential-6 potential for the two components results in more accurate predictions than Lennard-Jones potentials. Furthermore, Molecular Dynamics (MD) simulations were used to predict the diffusion coefficient of CO_2 in H_2O and of H_2O in CO_2 at subcritical and supercritical conditions [2,3]. Various combinations of force-fields were used that showed to provide results of different accuracy. Finally, MD and Monte Carlo (MC) simulations were used to predict density, vapour pressure, viscosity and interfacial tension of H_2O – NaCl mixtures. It was found that none of the examined models is able to predict all different properties with good accuracy [4].

Future work will be devoted to the development and validation of force fields that account explicitly for many body (polarizability) effects.

Acknowledgment

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IoLiCAP   **CO₂QUEST**

CO$_2$+SO$_2$ co-capture assessment. Part 1.

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Abstract

The concentration limits on the impurities of captured anthropogenic CO$_2$ for safe transport and injection as well as for the secure long-term geological storage have to be established analysing both aspects risk-safety and cost. When managing components hazardous to health and environment, for which removal can be expensive, co-capture may be an alternative approach.

SO$_2$ is one of the pollutants from power plants operations; the decision on its confinement along with CO$_2$ must be made by analysing the effects of this impurity on transport, injection and storage taking into account that the co-capture avoids its release into the atmosphere and the costs of purifying the exhaust gases. For this purpose we calculated and drew conclusions about the impact of SO$_2$ in the CO$_2$ on selected transport, injection, and storage parameters (minimum operational pressure, pipeline diameter and pressure drop, storage capacity, etc.), whose analysis is necessary for the safe construction and operation of CO$_2$ pipelines and for the secure long-term geological storage of anthropogenic CO$_2$. To calculate these parameters, it is necessary to acquire data on the volumetric properties and the vapor-liquid equilibrium of the fluid being subjected to CCS.

We present new and accurate experimental data of pressure-density-temperature-composition, P, ρ, T, x_{CO_2}, and vapor-liquid equilibrium, VLE, of five mixtures CO$_2$+SO$_2$ whose compositions range from x_{CO_2}= 0.8024 to 0.9930. Temperature and pressure ranges studied are of interest in CO$_2$ pipeline and geological storage sites, namely eight isotherms from 263.15 to 373.15 K and from 0.1 to 20 or 30 MPa. We have compared our experimental values in terms of relative mean deviation, MRD_X, with those calculated using PC-SAFT Equation of State [1, 2]. In addition, from this work and literature experimental data [3, 4], we have compared the effect of the presence of SO$_2$ and CH$_4$ in CO$_2$ evaluating several selected transport, injection and storage parameters.
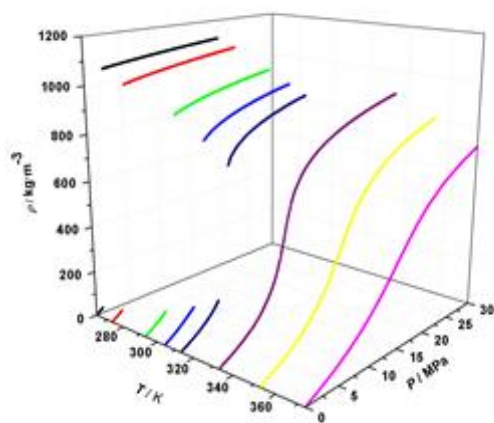
Figure 1. Experimental densities for the CO$_2$+SO$_2$ mixture with x_{CO_2}= 0.8969 at several temperatures and pressures.
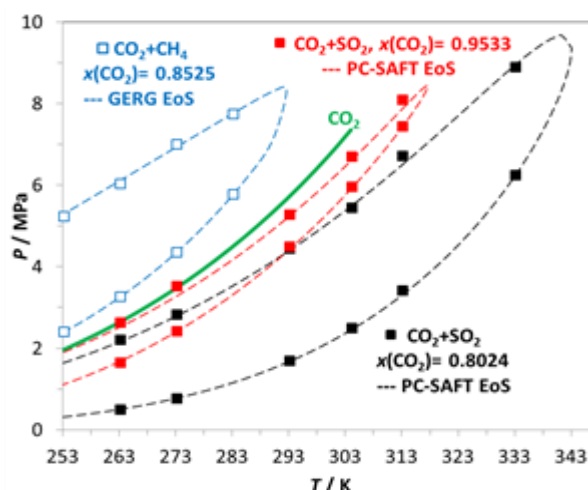

Figure 2. Experimental (this work and [4]) and predicted [1, 2, 5] phase envelopes for CO$_2$+SO$_2$ and CO$_2$+CH$_4$ mixtures, and vapour pressure of CO$_2$ [3].

Figure 1 shows the P, ρ, T experimental results for the CO$_2$+SO$_2$ mixture with x_{CO_2}= 0.8969. From 263.15 K to 313.15 K, the isotherms are subcritical and draw the VLE. The highest temperatures, from 333.15 K to 373.15 K, are supercritical isotherms whose slopes diminish as T increases.

As it can be seen in Figure 2 the presence of SO_2 reduces the bubble pressure of the mixtures, then the fluid can be transported at lower pressures than pure CO_2 or CO_2+CH_4 mixtures. The higher density of the CO_2+SO_2 mixtures results in a higher mass flow through the pipeline (Figure 3) and a lower pressure drop (Figure 4). The overall result is a lower number of booster stations or lower booster power requirements.
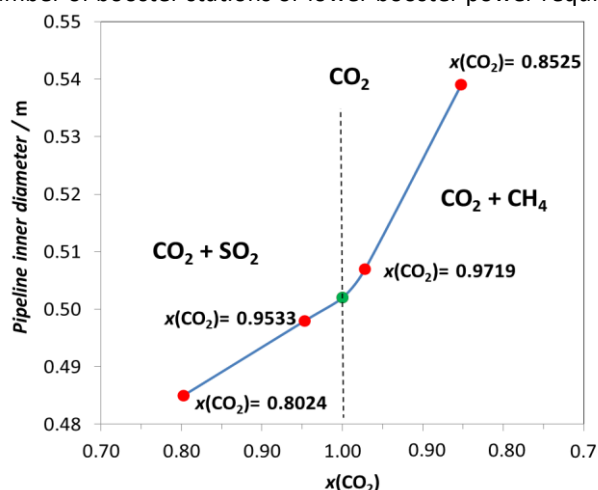

Figure 3. Pipeline inner diameter needed to transport 10 Mt/year of fluid at 10 MPa and 293.15 K.
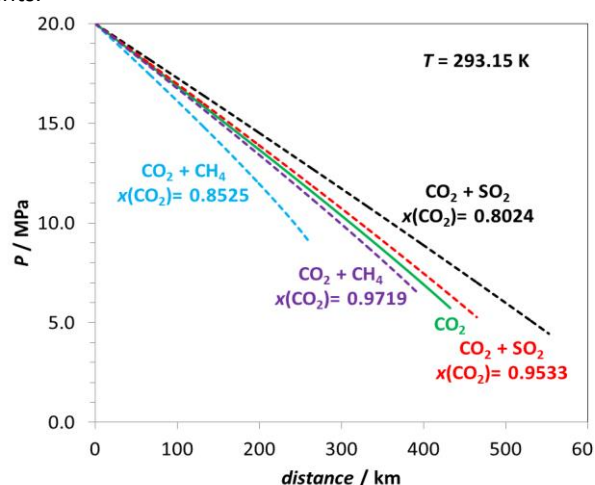

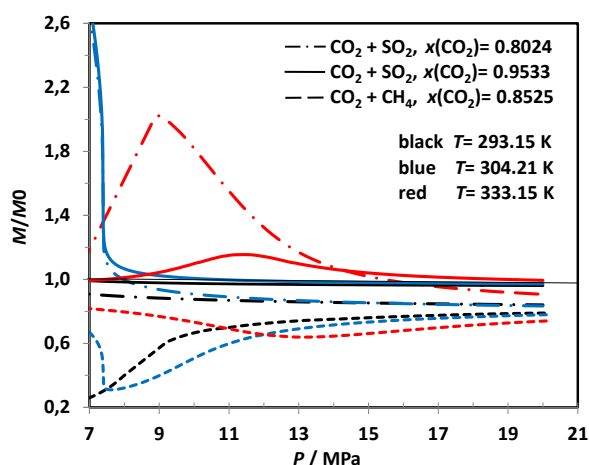Figure 4. Comparison of the pressure profile along a 20 inch - 10 Mt/year pipeline (this work, [3] and [4]).

Figure 5. Normalized storage capacity, M/M_0 (related to CO_2), for several CO_2+SO_2 and CO_2+CH_4 mixtures (this work and [4])

The presence of SO_2 affects positively the mass of anthropogenic CO_2 that can be stored in a reservoir (Figure 5), leading to the need for smaller storage capacity reservoirs and /or a lower number of sites to confine the same mass of fluid.

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A Global Overview of CCS Implementation

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Abstract

The IPCC's 5th Assessment Report (AR5) has set out a strong case for the need for Carbon Capture and Storage (CCS) as part of global efforts to mitigate greenhouse gas emissions and in particular CO2 emissions. The importance of CCS in the AR5 cannot be hidden, both for reducing emissions from fossil fuels and also for combining with bioenergy to take CO2 out of the atmosphere (BECCS or BioCCS). The report also shows that removing CCS from the mix will increase mitigation costs by a massive 138%, and may not achieve a 450ppm scenario at all. This is by far the highest increase from any of the technologies analysed (bioenergy, wind, solar, nuclear). "Note that many models cannot reach concentrations of about 450 ppm CO2eq by 2100 in the absence of CCS". So we really do need CCS in the portfolio of low carbon energy technologies. CCS also has benefits for the fossil fuel producers, where the report points out that the availability of CCS would reduce the adverse effects of mitigation policies on the value of fossil fuel assets.

CCS implementation has been moving more slowly than some of the other low carbon technology options but there is increasing activity in this area. The first CCS demonstration plant in the power sector was commissioned and began operating in October 2014. This was the SaskPower Boundary Dam3 project in Saskatchewan Canada. This is an 110MWe refit of an existing lignite fired boiler with post combustion capture technology. Other projects in the power sector such as Company's Kemper County Energy Facility in Mississippi USA are now under construction. Operated by Mississippi Power, it is planned to be fully in-service in the first half of 2016, when it will become the world's second commercial-scale coal power CCS project) and the world's first based on IGCC technology. As an IGCC, this is a polygeneration facility, not just a power plant. It will produce and sell 582 MW of electricity, 3 million tonnes pa of CO_2, 135,000 tonnes pa of sulphuric acid and 20,000 tonnes pa of anhydrous ammonia.

CCS implementation is not limited to the power sector, the Air Products steam methane reforming project in Texas USA has been operating for over a year now and has delivered over 1 million tonnes of CO**2** for EOR operations. Also in the H_2 production area we have the Tomokomai project in Japan and the Quest project IN Canada both under construction.

We should not forget that the first CCS demonstration project took place as long ago as 1996, the Sleipner project in the North Sea which has been injecting CO_2 successfully for over 20 years now. This was followed by two similar gas processing projects In-Salah in Algeria and Snohvit in the Barents Sea. The next project in this sector to come on board will the Gorgon project in Western Australia which will be the largest injection project in the world, injecting at a rate of 4MT/u year CO_2.

A new offshore EOR project started this year, the Lula project in Brazil, which combines capture from a gas processing facility with injection in the deep offshore for CO2-EOR operations. In the United Arab Emirates the Ramallah project involves the capture of CO2 from the Emirates Steel Factory in Abu Dhabi and its transportation to the ADNOC reservoirs for the purpose of enhanced oil recovery (EOR).

It is clear that with high oil process CO2-EOR was a driver in developing many of the CCS demonstration projects we see today. In Indonesia there is planes to develop a CO2 injection pilot to gain expertise in handling CO2 for future CO2-EOR operations. China has some 12 pilot projects underway that use CO2 for EOR operations and there are long term plans to develop large on shore EOR projects in China based on capture CO2 from planned coal to liquid, natural gas and fertiliser plants in Northern China.

In Europe CO2-EOR is not the driving force, it was planned that the ETS would provide support for CCS demonstration projects but that has not happened. Currently only the UK is pushing ahead with implementing CCS projects. There are two projects based on CO2 capture at a gas fired power plant in Scotland and a proposed oxy fuel project (White Rose) in Northern England. With the current demise of FutureGen 2.0 in the USA both these projects will be first of a kind technology demonstrations. Top enable such projects the UK has undertaken a reform of its energy market to provide project developers with investment confidence through the provision of long term supply contracts whilst protecting the consumer from significant electricity price increase.

A Geochemical Database for Subsurface Applications – theory and experiments

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Abstract

Reactive Transport Modeling (RTM) is the link between geochemistry and fluid transport in order to model multiphase fluid rock interactions in the subsurface. Shell's RTM capabilities comprises the in-house reservoir simulator MoReS (Regtien et al. 1995) which has been coupled to the open-source PHREEQC (Parkhurst & Appelo, 2013) chemical modeling platform. Such development in reservoir simulation enables Shell to model Carbon Capture and Storage (CCS) scenarios, well integrity and enhanced oil recovery (EOR) processes in taking into account mineral dissolution and precipitation, complexation and cation exchange mechanisms (Wei, 2012). Special emphasis has been put on the sequestration of contaminated gases in recent years to predict and therefore ensure safe containment up to a period of >10.000 years. Acid gases are corrosive in the presence of water and change dramatically pH and redox conditions which cause mineral dissolution and re-precipitation of secondary minerals. In addition, co-injection of certain impurities like SO_2 and NO_2 can enhance mineral dissolution in forming stronger acids in the presence of water under oxidizing conditions which impacts on CO_2 storage conformance. These reactivities enlarge the chemical systems to be taken into account for accurate reactive transport modelling in the subsurface. The reactivity of the injected fluids potentially can affect safe containment by changing cap rock integrity or influencing injectivity by changing porosity and permeability within the containment area. Therefore, it is of utmost importance to the operator and regulator to quantitatively understand fluid rock interactions during such projects. In order to accurately model and solve chemical batch reactions during the simulation, chemical equilibrium data for various minerals, chemical complexes and dissolved species need to be covered at a range of subsurface pressure and temperature conditions. The adequacy and accuracy of such an underlying thermodynamic database directly affect the outcome of the geochemical model. Therefore, it is essential that the database is continuously revised, extended, and benchmarked against available experimental data. For solid-liquid-equilibria (SLE), the standard computational tool and thermodynamic data package is the SUPCRT92 (Johnson et al. 1992) program which makes use of the Helgeson-Kirkham-Flowers(HKF) semi-empirical model of pressure and temperature dependences of equilibrium constants. OLI Systems with a solid foundation of simulating multi-component, electrolyte based chemical systems, has extended its thermodynamic database based on the revised HKF model and coupled its simulation capability to various activity models of which the mixed solvent electrolyte (MSE) model is the most recent and ubiquitous applicable one (Anderko et al. (2002). OLI Systems software suite links already to well-known Chemical Process Simulators (i.e. ASPEN, Unisim) and has a history in developing new chemical modules. We developed a link to transform OLI Stream Analyzer databases to PHREEQC in order to make use of its thermodynamic constraints within reservoir simulation. Here, we present an overview of relevant mineral systems in reservoir rocks, comprising saline aquifer and depleted oil/gas field, in the context of acid gas (CO_2/H_2S) sequestration. The aim is to identify potential thermodynamic knowledge gaps in these systems and make efforts to improve the database for these systems. The primary focus of our comparison is the carbonate and sulfate mineral system which is prone to react with dissolved CO_2 species in the subsurface. Experimental data from various literature sources and some of our own data are shown in comparison to predictions from OLI and MoReS-PHREEQC batch simulations. Finally, we give an overview of the prediction of the fate of injected CO_2, based on a range of reservoir simulation cases taking into account thermodynamic/kinetic uncertainties and other subsurface uncertainties.

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Potential Impact of Selected Impurities on Geochemistry

Related to CO$_2$ Storage

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Abstract

Typical impurities included in CO$_2$ streams captured from flue gas comprise compounds such as N$_2$, O$_2$, Ar, CO, SO$_2$, NO$_x$, H$_2$, or H$_2$S. They exert physical as well as chemical impact on the state of the geological reservoir, i.e. pressure, temperature, and salinity of brine in the target formation. Changes on density, buoyancy, and viscosity are dominated by N$_2$, Ar, and O$_2$. Whereas predominantly chemical effects are based on impacts of acidity, e.g. SO$_2$, H$_2$S, NO$_x$, in addition to changes of the redox state of the mineral-brine system, e.g. CO, H$_2$, O$_2$ [1, 2].

In order to study the extent of the geochemical impact, particularly competing chemical processes, reactive transport simulations were performed, using the thermo-hydrological-chemical code TOUGHREACT V3-OMP [3, 4]. The model is based on a one dimensional radial injection of CO$_2$ including 1 % SO$_2$ into a saline aquifer structure based on field data from the pilot site Heletz, Israel [5]. Of special interest were the effects of different time scales of transport versus aqueous chemistry, compared to mineral reactions.

For instance, SO$_2$ reacts with the formation water leading to sulphurous acid and the chemically important sulphuric acid under the local redox conditions, especially in case of an oxidative environment. Certain typical conditions may result in a particular residence time of SO$_2$ in the order of magnitude of those of advection, which allows transport to become a competing process. Hence, those conditions, in conjunction with the temporal evolution of the CO$_2$ plume, have a direct impact on the spatial distribution of the SO$_2$ dissolution, refer Figure 1. This yields a radius of influence of SO$_2$, which can be either strongly localised, associated with high acid concentration, or widely spread with low chemical impact. Consequently, a special focus is given to the aqueous chemistry and its kinetics [6] under geological storage conditions. In summary, the actual chemical evolution of SO$_2$ in a geological reservoir may have a significant impact on the geochemical system and subsequently on important parameters such as porosity, permeability, and injectivity.
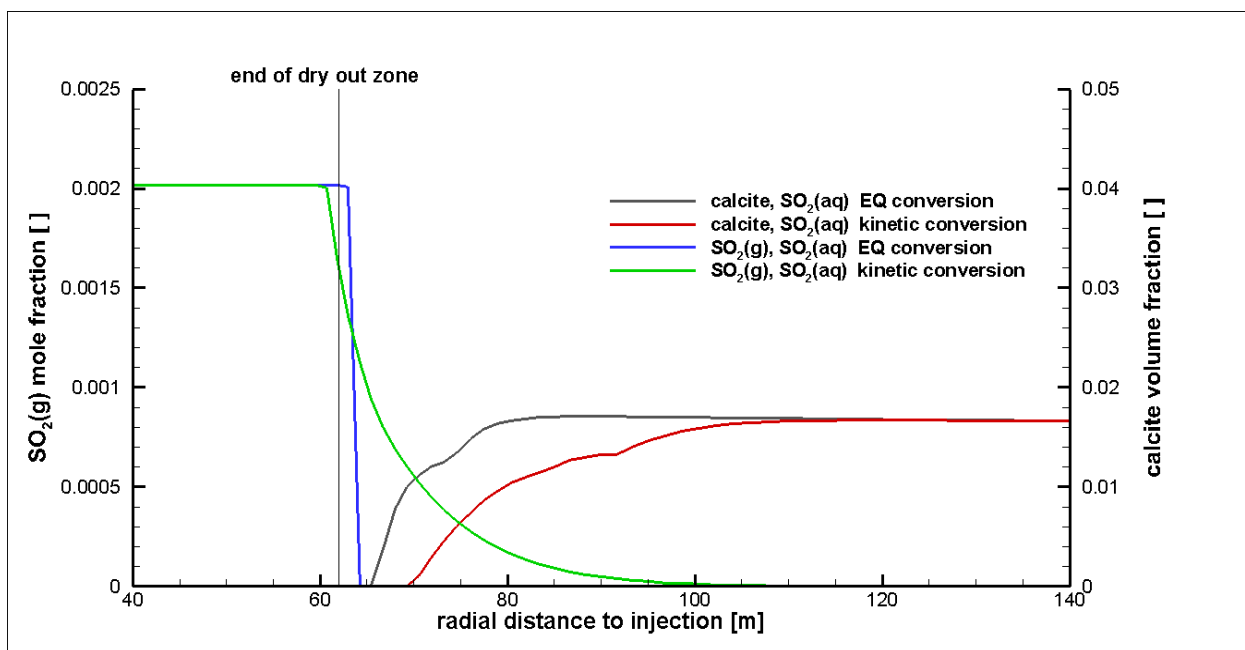
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Figure 1. Different radial extent of calcite dissolution due to larger spreading of $SO_2(g)$ in the gas phase, if conversion of $SO_2(aq)$ is calculated under aqueous kinetic constraint compared to equilibrium (EQ) constraint.

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The Plains CO$_2$ Reduction Partnership: Demonstrating Carbon Dioxide Storage in the United States and Canada

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Abstract

The Plains CO$_2$ Reduction (PCOR) Partnership is one of seven regional partnerships awarded in 2003 by the U.S. Department of Energy's National Energy Technology Laboratory to determine the best approaches to geologic storage and apply technologies to safely and permanently demonstrate the storage of carbon dioxide (CO$_2$). The PCOR Partnership region covers an area of over 1.4 million square miles in the central interior of North America and includes all or part of nine U.S. states and four Canadian provinces.

As part of the PCOR Partnership effort, a number of industrial partners have joined the program to undertake commercial-scale CO$_2$ storage projects, regional characterization efforts, and large-scale CO$_2$ storage project feasibility studies. Currently in the eighth year of the demonstration phase, the PCOR Partnership is testing the validity of different characterization, modeling and simulation, risk assessment, and monitoring techniques and technologies to advance the science of CO$_2$ storage in geologic formations. Completed efforts to date include a best practices manual for a feasibility study surrounding the potential to inject over 2 million tonnes of CO$_2$ a year near Spectra Energy's Fort Nelson Gas-Processing Plant [1, 2]; the completion of an updated regional technology implementation plan surrounding Apache Canada's Zama acid gas enhanced oil recovery (EOR) and CO$_2$ storage project [3]; and a binational effort between the United States and Canada to characterize the lowermost saline system (basal Cambrian) in the Williston and Alberta Basins [4]. In addition to the completed efforts, there are several ongoing efforts, including injection at the Bell Creek project and planned injection (scheduled to begin in 2015) at the Aquistore project.

The PCOR Partnership is collaborating with Petroleum Technology Research Centre (PTRC) in site characterization; risk assessment; public outreach; and monitoring, verification, and accounting (MVA) activities at the Aquistore project. The Aquistore project is a carbon capture, utilization, and storage (CCUS) project situated near the town of Estevan, Saskatchewan, Canada, and the U.S.–Canada border. This project is managed by PTRC and will serve as buffer storage of CO$_2$ from the SaskPower Boundary Dam CCUS project, the world's first commercial-scale postcombustion CCUS project from a coal-fired electric generating facility. In early 2015, CO$_2$ captured from SaskPower's Boundary Dam power facility will be transported to the Aquistore site and injected into the Deadwood Formation for long-term CO$_2$ storage [5, 6].

At Bell Creek, the PCOR Partnership is working with Denbury to study CO$_2$ storage associated with commercial CO$_2$ EOR at the Bell Creek oil field. The Bell Creek oil field covers approximately 22,000 acres (89 square kilometers), contains over 450 wells, and has produced over 130 million barrels of oil since its discovery in 1967. Denbury is injecting approximately 50 million cubic feet (1.4 million cubic meters) of CO$_2$ a day, sourced from from the ConocoPhillips-operated Lost Cabin Gas Plant and the ExxonMobil Shute Creek Gas Plant in LaBarge, Wyoming. The CO$_2$ is being transported to the Bell Creek oil field via the 232-mile (373-kilometer)-long Greencore pipeline and injected into an oil-bearing sandstone reservoir in the Lower Cretaceous Muddy Formation at a depth of approximately 4500 feet (1372 meters) for the purpose of CO$_2$ EOR. Denbury is carrying out the injection and production operations, while the EERC is providing support for site characterization, modeling and simulation work, integrated risk assessment, and aid in the MVA of the injected CO$_2$ [7, 8]. Injection operations began in the Bell Creek Field in May 2013 and as of the end of August 2014, 1,247,174 tonnes of CO$_2$ had been injected.

The PCOR Partnership also continues to provide widespread carbon capture and storage outreach and education, aid in regulatory development, and collaboratively undertake regional characterization efforts [9]. Paramount to the PCOR Partnership efforts is knowledge-sharing focused on concepts and techniques that have proven effective for the implementation of large-scale CO$_2$ injection projects. Discussion will focus on lessons learned and strategies that were

successful in the feasibility, design, and/or implementation phases of projects with PCOR Partnership Program involvement.

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Predicting the long-term fate of the stored CO$_2$: main findings of the EU-FP7 funded PANACEA

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Abstract

The ability to predict the long-term fate of the stored CO$_2$ is of key importance in many aspects of the CO$_2$ storage, design and planning as well as certification. The EU-FP7 funded PANACEA project has investigated many aspects of the problem. The project started on January 2012 and ended on December 2014. The project consortium comprised 12 partners (EWRE- coordinator, Israel Institute of technology, Uppsala University, University of Gottingen, CSIC of Spain, CNRS – Montpellier of France, Edinburgh University (Scotland), Cambridge University (UK), Statoil (Norway), Nottingham University (UK), IMAGEAU (France) and BUREAU VERITAS (France).

The aim of PANACEA was to contribute to a reliable prediction of the long-term fate of the stored CO$_2$ and to develop the tools required for the transition from research and development activities to large-scale, industrial, deployment of CO$_2$ storage. In PANACEA, we developed methods and tools for improved prediction and validation of the long-term behavior of stored CO$_2$. The project consisted in an extensive effort of model development and application and validation on a number of sites: EEPR funded Hontomin (Spain), EU-FP7 funded Heletz (Israel) and Sleipner (Norway), for the quantification of key impacts subsequent to the storage of CO$_2$. International cooperation has been set with major CCS research centers in the USA, Canada and Australia.

In order to achieve this goal we defined five inter-related objectives:

- Identify and quantify the factors responsible for the long-term stability of the stored CO$_2$.
- Provide measures for the assessment of the integrity and vulnerability of the reservoir (storage formation and cap-rock) and wells that penetrate it, to the CO$_2$ stream.
- Quantify the impact of the stored CO$_2$ on adjacent subsurface reservoirs as changes in the reservoir (in pressure, pH, and chemical reactions) may lead to unwanted migration of brines and release of pollutants trapped in the rock to freshwater reservoirs.
- Identify and develop reliable monitoring, measurement and verification (MMV) technologies having the capacity to capture relevant information on the long-term behaviour of the stored CO2 both at the near and far field (new ERT probe).
- Achieve an adequate degree of cooperation with projects and initiatives in order to allow the collection of data necessary for validating the investigations and to allow the dissemination of findings.

Numerous relevant results have been achieved so far and over 50 peer-reviewed papers. Below are outlined a few of them (due to space reporting limits):

- Improved prediction of the CO$_2$ spreading at Sleipner, matching the measurements obtained from seismic surveys and modelling efforts, which so far have not able to satisfactorily predict the CO$_2$ plume migration (Figure 1).

- Simplified tools for the prediction of the regional pressure build-up (pressure plume) subsequent to storage of CO_2 for fast prediction of near field and far field environmental impacts. We were able to predict with relatively very simple (fast) models, the pressure behaviour CO_2 storage predicted by very sophisticated (slow) ones.
- Simplified analytical solutions for the prediction of CO_2 leakage, spreading and trapping via convective dissolution, using very simple geometries. These allow a preliminary analysis of a potential site, prior to any exploration and or characterization activities.
- Understanding the CO_2 trapping from the analysis of natural analogues and construction of computational models for the simulation of CO_2 migration in one analogue reservoir, using three different simulators (for cross-model comparison).
- Understanding reactivity of CO_2 with regard to rock matrix and cement (laboratory work).
- Predicting leakage rates of CO_2 through faults. A model was constructed, using LBNL ECO2M, from the reservoir to the ground level and the migration of CO_2 was simulated through faults, including phase change and dissolution in the fresh water layer. Under the assumptions of the model, results show that in case of leakage, the total mass of leaking CO_2 is negligible.
- Developing and prototype testing (at Maguelone, France) of the integrated RSTG (Resistivity, Seismicity, Temperature and Gas sampling), station, to be deployed using a "behind the casing " non-perforated wells.
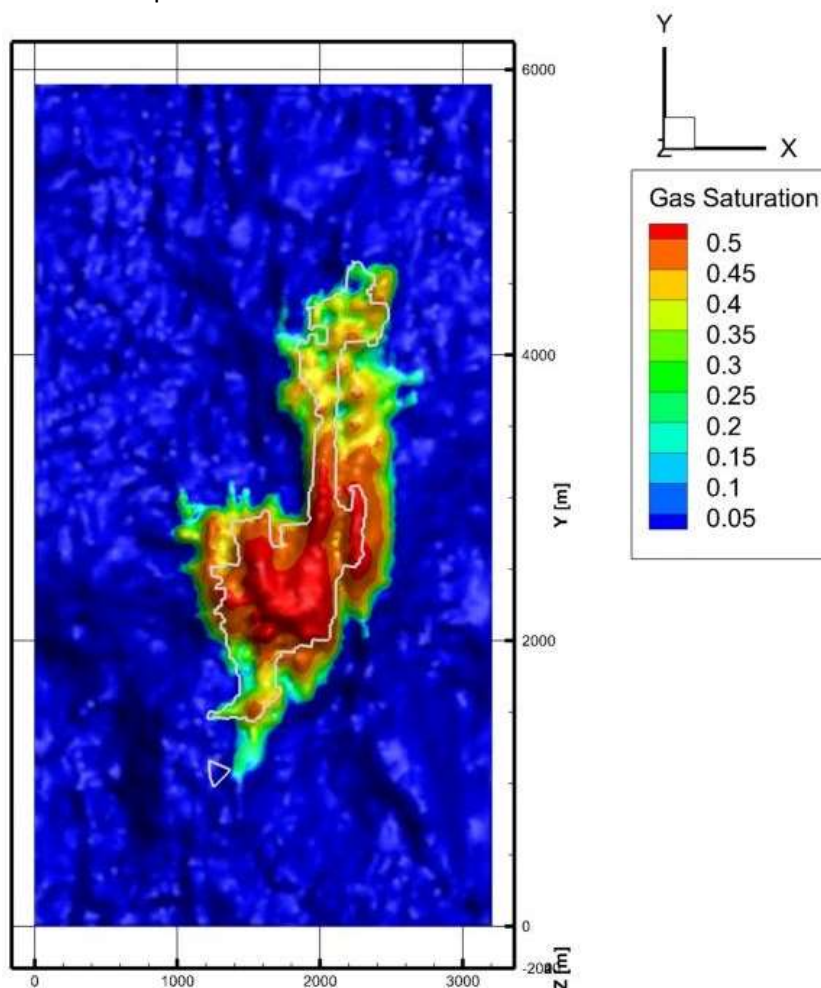

Figure 1: CO_2 plume (color) top view vs. survey (grey), year 2008 (last year of publicly available data).

Numerical modelling of dynamic brittle crack initiation and propagation of pipeline steel

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Abstract

Crack initiation and propagation in pipeline steels is usually evaluated by means of Charpy impact test. The Charpy test, also known as the Charpy V-notch test, is a standardized high strain-rate test which determines the amount of energy absorbed by a material during fracture. Tests are performed in a wide temperature range (-120°C up to RT) to construct the transition curve. At elevated temperatures (upper shelf region) the fracture is almost fully ductile, while in the lower shelf region, a brittle fracture can be observed.

In general one can distinguish between two approaches to study fracture mechanics: the global approach and the local approach. In the global approach, it is assumed that the resistance to fracture can be measured in terms of one single parameter, for example the critical stress intensity factor. This approach, however, does not account for the microstructure of the material, while there is sufficient experimental evidence to assume that several microstructural features affect the occurrence of brittle fracture: carbide particles, Martensite-Austnite constituents, crystallographic texture, etc.

In this investigation the local approach is adopted by means of eXtended Finite Element Method (XFEM)-based cohesive zone modelling approach to simulate dynamic crack initiation and propagation of pipeline steels at low temperatures. For this purpose, crack initiation refers to the beginning of degradation of the cohesive response at an enriched element, where the initial crack occurs if the principal stress exceeds a critical value in front of the crack tip. Once the corresponding initiation criterion reaches, XFEM crack advances through enriched cohesive elements by means of traction-separation constitutive behaviour up to final rupture of the test sample. In terms of mixed mode crack propagation, when the maximum principal stress criterion is specified, the newly introduced crack is always orthogonal to the maximum principal stress direction when the fracture criterion is satisfied. The numerical cohesive zone damage parameters are calibrated using studying the fracture behaviour of Single Edge Notch Bending (SENB) specimen at low temperatures. The results highlight the capability numerical modelling approach which may be used as a basis for revision of existing design methods of pipelines integrity.

CO$_2$ compression and flow in transportation networks

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Abstract

The accurate design and economic evaluation of a suitable high-pressure CO$_2$ pipeline transportation networks, which will be employed as part of any Carbon Capture and Sequestration (CCS) project, requires the availability of reliable pipeline thermo-hydraulic models. In the present study, performed as a part of CO2QUEST project [1], the accuracy of several thermo-hydraulic models currently used in industry is assessed by comparison of their predictions of the fluid temperature and pressure drop in the pipeline transporting supercritical CO$_2$ against those obtained from a rigorous model of one-dimensional steady-state flow in a pipe. The latter model is based on on-dimensional conservation equations of mass, momentum and energy accounting for the viscous friction and heat transfer through the pipe wall [2, 3, 4] and nonlinear variation of the physical properties of supercritical CO$_2$ fluid with pressure and temperature. The study is performed for a 0.8 m internal diameter horizontal pipeline transporting CO$_2$ over distances from 10 to 40 km using buried, insulated and non-insulated above-ground pipelines operating at pressures from 80 to 170 bar and temperatures between 20 and 60 ^{o}C.
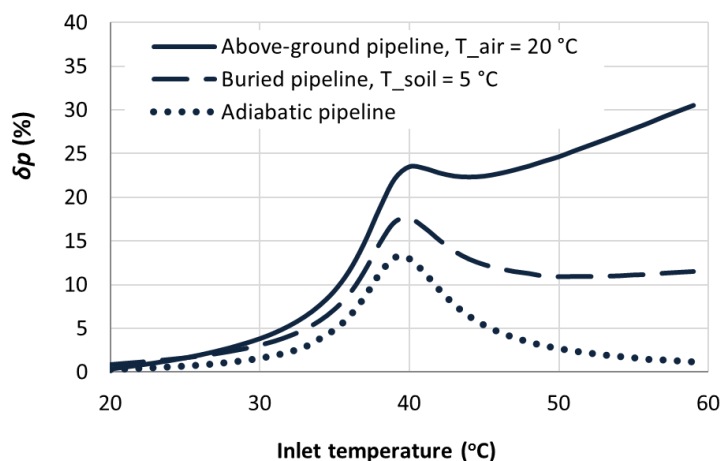
Figure 1. Impact of pipeline inlet temperature and insulation conditions on the relative difference in the pressure drop predictions obtained using the Darcy-Wesbach equation and the rigorous one-dimensional flow model. Pipeline length is set to 20 km, pipeline diameter is 0.8 m, the inlet pressure is 90 bar and the inlet velocity is 3 m/s.

Figure 1 shows an example of calculation of the discrepancy between the pressure drop predictions using a thermo-hydraulic model based on Darcy-Weisbach equation and the rigorous one-dimensional flow model. The results presented in Figure 1 were obtained for various inlet temperatures and different pipeline insulation conditions, assuming the pipeline is 20 km long, has internal diameter of 0.8 m and transport pure CO_2 at inlet pressure of 90 bar and inlet velocity 3 m/s. As can be seen from Figure 1, in the case of the above-ground uninsulated pipeline the inaccuracy of the thermo-hydraulic model predictions can reach *ca* 30 % at the inlet temperatures above *ca* 40 ^{o}C. Such large overestimation of the pipeline pressure drop can lead to substantial overdesign of the pipeline, which may involve using thicker-wall pipes and larger number of compressor/ pump stations along the pipeline route than necessary.

To simulate operation of a large CO_2 transmission pipeline network, the differential steady-state flow model of flow in a pipeline was further extended to account for mixing of streams from multiple sources into a single stream transported to a geological storage location. This model is being applied to study the impact of variation in the CO_2 stream impurities fed into the pipeline network at different points, upon the pressure and temperature profiles along the network and the delivery composition for a given flow-rates and temperatures of the feed streams. For a hypothetical pipeline network configuration the analysis of the steady-state pressure drop and temperature profiles has been performed for CO_2 mixtures carrying various impurities, including water, argon, nitrogen and oxygen, which are typically present in the oxy-fuel combustion CO_2 stream. The computational model developed provides a useful tool for sensitivity studies aiming to identify impurities having the most adverse impact on the CO_2 pipeline transport.

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Impact of impurities on pipeline specification and hydraulics

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Abstract

The purity of the CO2 stream emitted from carbon capture plants is extremely important for the design and operation of CO2 pipelines, affecting, amongst other things, the hydraulic efficiency and potential operating range as well as having implications for the safety and integrity of the pipeline system. However, to date, there is still uncertainty regarding the range of impurities that could enter the transport and storage systems for Carbon Capture and Storage (CCS) schemes. The main difficulty in being able to specify a CO2 pipeline composition is that the type and levels of potential impurities in the CO2 stream will differ between power plants and industrial sources and also between the capture technologies installed at the sources. The problem is further compounded by the fact that, not only does each impurity cause different effects on the transportation system, these effects, for any individual component, can vary with conditions and can, for example, alter gaseous and dense phase pipeline operation in different ways. Additionally, the mixtures of impurities in CO2 streams leaving different capture processes could vary substantially, leading to dramatically different effects on compression, transport and storage operations.

This paper investigates the effects of impurities on pipeline sizing for dense phase and gaseous phase pipeline transportation using a series of twelve CO2 impurity scenario compositions. The scenarios have been selected as worst-case compositions that are representative of plausible CO2 streams from different capture technologies and industry sources. Two analyses are presented:

i)   an initial hydraulic analysis, conducted for a single point-to-point pipeline transporting a fixed flow rate of CO2 in either the dense phase or gaseous phase and

ii)   a sensitivity analysis to evaluate the effects of inlet pressure, ambient temperature and mass flow rate and pipeline size and identify an optimum pipeline size to handle each scenario in a hydraulically efficient manner.

The inlet and outlet temperature and pressure ranges for each pipeline were selected based on a detailed analysis of the thermodynamic properties of the different streams, which is also discussed. As a result of the study, conclusions are drawn regarding the compositions that present the most challenge with respect to hydraulic efficiency and pipeline costs. In addition, guidance is provided on the specification of inlet conditions to improve the hydraulic performance of the pipeline.

This work forms part of a study supported by IEAGHG on the "Impact of CO2 Impurity on CO2 Compression, Liquefaction and Transportation". The study was commissioned to identify potential impurities and address the consequences of their impact on CO2 transportation. The study is still in progress and currently under peer review.

Effect of Ionic Liquids with Imidazolium and Lactam-Based Cations on Corrosion of Mild Steel

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Abstract

Ionic liquids (ILs) have been extensively investigated during the last decade due to their unique physicochemical properties and diverse potential applications. Industrial applications of ILs require understanding of their interactions with metallic materials used for construction of installations that contain IL-based environments. Here, the corrosion behaviour of mild steel (MS) in ILs exclusively developed for post-combustion CO_2 capture processes by IoLiTec Ionic Liquids Technologies GmbH is reported.

Two 1-alkyl-3-methylimidazolium tricyanomethanide (TCM) ILs (alkyl=butyl and hexyl) and one butyrolactam cation-based IL with a fluorinated anion, pyrrolidium-2-one bis[(trifluoromethyl)sulfonyl]imide ([BHC]BTA), were synthesised and tested in contact with MS at temperatures up to 80 °C. The corrosion behaviour was evaluated by monitoring the morphological changes on the steel surface after testing. Exposure of MS to the IL results in two main types of degradation that depend on the IL type and include the following: (i) local changes on the surface at the locations of MnS inclusions present in the steel and (ii) modification over the macroscopic surface of the alloy.

The 1-alkyl-3-methylimidazolium TCM ILs promoted dissolution of MnS inclusions. In the ILs with a shorter alkyl chain in the cation (alkyl=butyl), the dissolution of MnS was accompanied by generation of corrosion products around the inclusion sites, which are mainly identified as magnetite and maghemite ferrites [1] (Fig. 1 (a)). No corrosion products were generated in the IL with hexyl in the cation that was attributed to the increase of the inhibition ability of the IL with the longer alkyl chain of the cation (Fig. 1(b)). The rest of the macroscopic steel surface remains unaffected. It should be noted that the high inhibition ability of these ILs remains unaffected at relatively long-term immersion durations of 30 days that confirms their high stability.
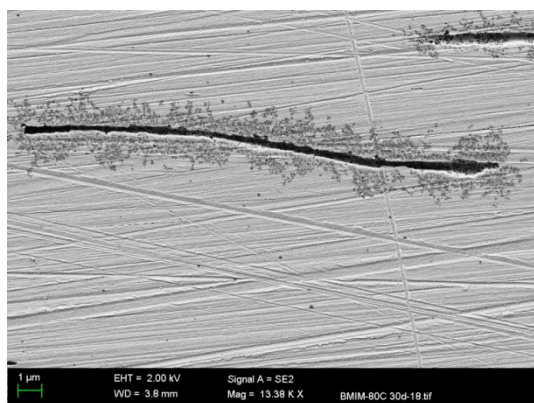
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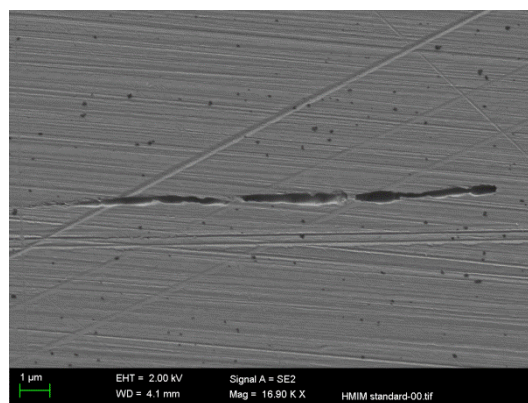
b

Figure 1. Scanning electron micrographs of mild steel after immersion testing in 1-alkyl-3-methylimidazolium TCM ionic liquids at 80 °C for 30 days: (a) alkyl=butyl; (b) alkyl=hexyl

General etching over the macroscopic surface of the alloy was revealed for the IL with the fluorinated anion. Etching resulted in significant weight loss due to removal of material, whereas no significant weight loss was revealed following MnS dissolution in the ILs with TCM anion. [BHC]BTA severely attacks MS with the formation of a plethora of corrosion products on its surface at 80 °C. General etching also occurs at room temperature; however, the amount of corrosion products on the surface is significantly reduced (Fig. 2 (a-c)). Microscopic examination of the surface of MS after immersion in [BHC]BTA reveals the presence of pearlite and ferrite phases (Fig. 2 (d)).

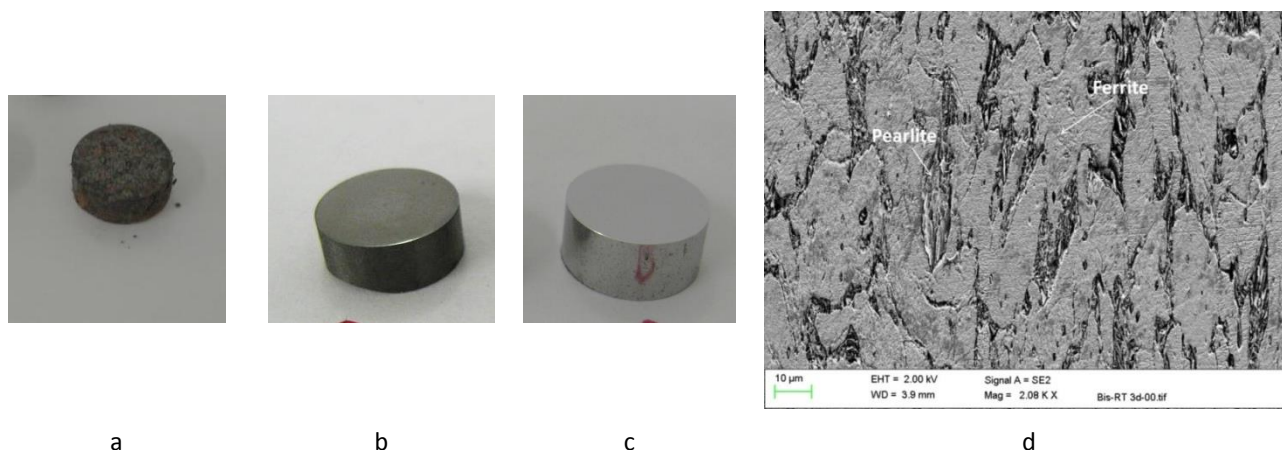a   b   c   d

Figure 2. Photographs of the mild steel specimens after immersion testing in [BHC]BTA: (a) 80 °C, 3 days; (b) room temperature, 3 days; (c) as-polished alloy. (d) Scanning electron micrograph of mild steel after immersion testing in [BHC]BTA at room temperature for 3 days

It was revealed that addition of 500 ppm sodium molybdate to [BHC]BTA resulted in efficient inhibition of etching at both room temperature and 60 °C due to adsorption of molybdate on the alloy surface (Fig. 3). XPS examination confirmed that the species with molybdenum in hexavalent state are adsorbed on the surface of MS, thus providing effective corrosion inhibition.

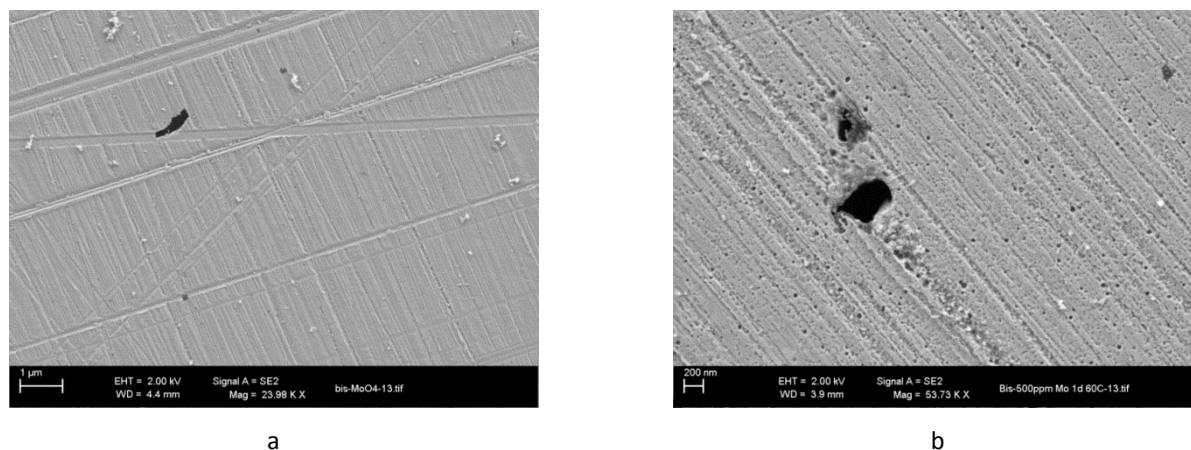
a   b

Figure 3. Scanning electron micrographs of mild steel after immersion in [BHC]BTA with added 500 ppm sodium molybdate at (a) room temperature for 3 days and (b) 60 °C for 1 day

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Transferring CCS Research into Good Transportation Design

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Abstract

Safety considerations are the most important aspect of designing new installations. In addition to the inherent risks of maintaining high pressure systems, large volumes of Carbon Dioxide (CO_2) present hazards that are becoming progressively better understood by the scientific community. Chief among these are the toxicity, high density and a change in the physical properties of CO_2 as the fluid is subjected to changes in process conditions.

Engineers need to work with scientists to transpose the emerging scientific knowledge into safe, reliable and efficient designs. By way of example, we consider here, how knowledge gained about the behaviour and characteristics of CO2 is playing a large part in the design of a fixed installation such as a CO_2 pumping station.

The Role of Degradation on Foaming of Various Amine Solvents in Model Columns

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Abstract

Amine foaming is a problem in post-combustion carbon capture. The existence of this phenomenon has been reported anecdotally and little research has addressed the behaviour. Industrially, the problem is mitigated by adding agents suspected to decrease the foaming. However, not only are these insufficiently effective in some cases but also cause additional problems. Limited work has been pursued in this field, but it has been previously suggested that clean amine solutions foam demonstrably less than those which are contaminated [1]. However, the bulk of work has been conducted on relatively clean amine solutions with some additional emphasis on anti-foaming additives. Previously, a comprehensive study [2] on monoethanolamine was conducted, to establish the role of variables in the foaming process. The work presented expands on that, to address the potential interactions amongst variables deemed most influential, and compare the outcomes in MEA and three popular alternative amines. This important study will provide the baseline for ongoing to address the foaming with respect to more industrially relevant complexities.

Figure 1. Model column.

Individual amine solvents were all used as received: monoethanolamine (MEA) (>98%, Sigma), methyldiethanolamine (MDEA) (>99%, Sigma), 2-amino-2-methyl-1-propanol (AMP) (>95%, Sigma), and 1-(2-aminoethyl)piperazine (AEP) (99%, Sigma). Solutions (100mL) for each amine solvent were prepared at 10 and 30 weight percent with de-ionized water and subsequently purged with nitrogen to avoid any oxygen contamination. Samples were then bubbled with carbon dioxide until the solution was saturated (overnight). This process was repeated with a second set of samples where air was bubbled into the sample overnight.
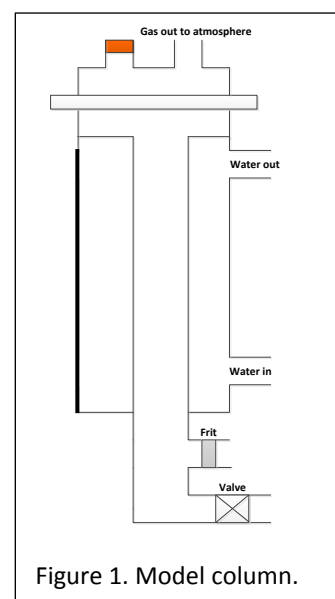
Run	Concentration (weight %)	Temperature (°C)	Nitrogen Flow Rate* (m/s)
1	10	55°C	7.0×10^{-4}
2	30	55°C	7.0×10^{-4}
3	30	85°C	7.0×10^{-4}
4	10	85°C	7.0×10^{-4}
5	10	85°C	7.0×10^{-3}
6	10	55°C	7.0×10^{-3}
7	30	55°C	7.0×10^{-3}
8	30	85°C	7.0×10^{-3}

Table 1: Experiments to understand the individual and combined role of amine concentration, temperature, and nitrogen flow rate on the development of foaming. *normalized to the cross-sectional area of the column

Experiments were designed on a simple 2^3 fractional factorial where the effects (variables) included amine solution concentration, temperature, and nitrogen flow rate during the experiment. Table 1 details the experimental conditions of each of the eight trials, run on both a 'clean' and degraded sample. This will therefore address not only the main effects, but also the interactions amongst them in degree of foaming.

Each sample solution was tested in a model column scaled to correlate with many columns used in pilot plants (and therefore larger-scale as well). A schematic is shown in Figure 1. A water jacket was used to control the temperature of the amine solvent. Gas was controlled with a flow meter and introduced through a frit to increase initial bubble dispersion.

Foaminess was measured using a method previously described [3], where it is a ratio of total steady volume of foam to the velocity of gas. Foam was measured for thirty minutes; after which breakthrough time was measured.

Under 'clean' (no oxygen) conditions, some foaming was observed in the solvents MDEA and AMP (Table 2 and 3, respectively). MDEA shows foaming only under higher flow conditions; this is determined to be the main effect controlling foam in this case. It must also be noted that there is a more minor contribution from the interaction of temperature with the other two variables. Interestingly, the foam predominantly forms under the same conditions when the solution has been degraded. However, an additional case is seen at lower flow rates when a combination of low temperature and concentration are implemented. This causes a stronger effect from temperature. The similarities in this case suggest that there is an intrinsic foaming behaviour in the MDEA that is less strongly influenced by its short-term degradation.

In the case of 'clean' AMP the main effect is strongly temperature. There is an additional more minor interaction from concentration with temperature. Interestingly, once the solvent degradation has taken place the lower temperature increases foaminess. This important differentiation demonstrates that the chemical changes in the solvent are strongly influencing the physical behaviors observed. Industrially this has significant importance, pointing to potential problems in the absorber.

Non-degraded amine solutions demonstrated significantly less foaming than their more degraded counterparts. The amine solvents MEA and AEP showed no foaming whatsoever under any of the eight conditions considered. These findings are similar to those previously seen [3]. More surprising is the lack of foaming by AEP where foaming was observed in piperazine [3]. With the introduction of air, MEA did show a significant increase in foaming (Table 4) whereas AEP did not. This finding again correlates to that previously reported [3] were iron (II) was added to induce oxidative degradation. In this work, the foaming observed in MEA was significant, and strongly influenced by the flow rate of nitrogen.

The comparison of foaming for MDEA, AMP, and MEA importantly shows that the three amine solvents do not exhibit the same foaming tendency when subjected to the same conditions. As a result it is clear that the foaming of amine solvents cannot be treated categorically but rather will require individual specifications. Additionally, the difference observed in influencing factors will be necessary in addressing this industrial complication. Previous work has suggested the role of degradation in foaming and here it has been conclusively shown. This work provides a strong basis for a continued study of foaming with more industrial complications.

Run	MDEA 'clean' Foaminess (m^2/s)	MDEA degraded Foaminess (m^2/s)
1	0	2.0×10^{-2}
2	0	0
3	0	0
4	0	0
5	3.3×10^{-3}	7.3×10^{-3}
6	3.3×10^{-3}	6.5×10^{-3}
7	1.4×10^{-2}	1.1×10^{-2}
8	0	0

Table 2: MDEA Foaminess

Run	AMP 'clean' Foaminess (m^2/s)	AMP degraded Foaminess (m^2/s)
1	0	0
2	0	1.6×10^{-2}
3	1.2×10^{-2}	0
4	0	0
5	6.7×10^{-3}	0
6	1.6×10^{-3}	1.5×10^{-2}
7	0	6.5×10^{-3}
8	1.2×10^{-2}	1.6×10^{-2}

Table 3: AMP Foaminess

Run	MDEA degraded Foaminess (m^2/s)	AMP degraded Foaminess (m^2/s)	MEA degraded Foaminess (m^2/s)
1	2.0×10^{-2}	0	1.5×10^{-2}
2	0	1.6×10^{-2}	1.7×10^{-2}
3	0	0	1.2×10^{-2}
4	0	0	8.1×10^{-3}
5	7.3×10^{-3}	0	5.7×10^{-3}
6	6.5×10^{-3}	1.5×10^{-2}	4.9×10^{-3}
7	1.1×10^{-2}	6.5×10^{-3}	4.1×10^{-3}
8	0	1.6×10^{-2}	3.7×10^{-3}

Table 4: MDEA, AMP, MDEA degraded Foaminess

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IoLiCAP   **CO$_2$QUEST**

Do Ether Functionalized Ionic Liquids Improve the CO$_2$ Solubility?

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Abstract

CO$_2$ absorption using a solvent is accepted as the most compatible technology. In the recent years ionic liquids (ILs) have shown to be good candidates for CO$_2$ capture. They exhibit major advantages compared to amine-based systems. Their negligible vapor pressure, high thermal and chemical stability and tunability outweigh the disadvantages of lower absorptive capacity and kinetics.

In this work a comprehensive study of the ILs [C$_2$mim]-, [C$_4$mim]-, [C$_6$mim]-, [C$_7$mim]- and [C$_8$mim] tricyanomethanide (TCM) has been carried out. Furthermore, in order to evaluate the presence of ether groups in the alkyl chain of the imidazolium, this work includes 1-(2-methoxythyl)-3-methylimidazolium- and 1[2-(2-methoxyethoxy)ethyl]-3-methylimidazolium tricyanomethanide. These non-flourinated and low-viscous ILs are studied for the first time as a solvent for CO$_2$ capture. Two different methods (volumetric vs gravimetric) were applied to study the thermodynamics (i.e., absorptive capacity and Henry's law coefficient) and kinetics (i.e., diffusion coefficient) at several temperatures and pressures up to 150 bars. The experimentally determined phase behavior of the IL and CO$_2$ systems are correlated using the Peng-Robinson equation of state. Furthermore, the thermal operating window (e.g., glass transition and decomposition temperature) and physical properties (e.g., density, viscosity, conductivity and surface tension) were determined.

It will be shown at the conference that TCM-based ILs are promising sorbents for pre-combustion CO$_2$ capture due to their high (physical) absorptive capacity, their low regeneration energy consumption (low heat of absorption) and improved kinetics (due to their low viscosity) compared to the conventional ILs.

IoLiCAP   **CO$_2$QUEST**

Up scaled synthesis of TCM-based ionic liquids for CO$_2$ capture

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Abstract

Ionic liquids (ILs) are defined as compounds consisting entirely of ions and being liquid at unusual low melting points, by definition below 100 °C. Due to the wide range of possible cation and anion combinations ILs offer tunable and unique mixes of properties, such as conductivity, viscosity, density, solubility, and high thermal and chemical stability. With these versatile properties they are promising candidates for various applications such as CO$_2$ capture.

The current process to capture CO$_2$ is based on aqueous amine solutions, which are volatile and also highly corrosive. Due to their ability to retain CO$_2$ - both physically (physical sorption) and chemically (chemisorption)[1] - ILs can be used for the direct capture of CO$_2$. Two great benefits of the application of ionic liquids for CO$_2$ capture are the reduction of solvent release to atmosphere due to their ultra-low vapor pressure, and a reduced corrosion of plant components by usage of specially designed IL candidates. At the same time an elevation of absorption/stripping rates and CO$_2$ loading can be achieved.

In our work, we synthesized numerous ionic liquids and conducted first screening tests in order to investigate their behaviour concerning CO$_2$ absorption, corrosivity, and ecotoxicity. After a couple of iterations and optimization procedures, we identified a mixture of three suitable candidates for further testing in a pilot plant[2]. Also in view of a potential industrial use of these ILs, we developed a synthesis strategy using continuous flow techniques.
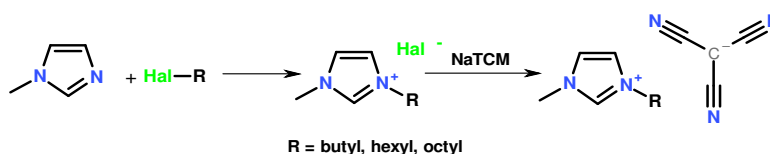
R = butyl, hexyl, octyl

Figure 1. Synthesis of tricyanomethanide-based ionic liquids

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On the Use of Ionic Liquids in Order to Inhibit/Promote CO$_2$ Hydrates

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Abstract

The capture and subsequent sequestration of CO$_2$ has been suggested as a possible solution in reducing the amount of the particular green-house gas from the atmosphere. In a number of studies the authors have considered the use of ionic liquids (IL's) as part of the capture process.

Motivation for the current study is the use of gas hydrates in a number of practical applications. In particular, gas hydrates are encountered in a number of applications of industrial and scientific interest. Of significant interest are the cases of flow assurance, gas storage and transportation, and gas mixture separation. All three cases are of relevance to the problem of capture and sequestration of CO$_2$. Under moderate pressure and temperature conditions CO$_2$ hydrates can form. Therefore, during the transportation of CO$_2$ through pipelines, if H$_2$O is present as well, and the temperature and pressure conditions are appropriate, crystalline hydrates can form. Hydrate formation can result in pipe-line blocking which is considered a serious industrial problem. As a result, either H$_2$O has to be removed from the flow lines or hydrate inhibitors need to be added. IL's have been identified as potential inhibitors.

When a substance is added in a hydrate-forming system the hydrate formation can become more difficult (i.e., hydrate inhibition) or easier (i.e., hydrate promotion). The first case is essential to the transportation of CO$_2$ through pipelines, while the second case is essential for designing capture processes for the separation of CO$_2$ from flue (CO$_2$ + N$_2$) or fuel (CO$_2$ +H$_2$) gases.

In the current study we perform: (i) a theoretical analysis for CO$_2$ hydrates in the presence of IL's, and (ii) a series of experimental measurements where the performance of different IL's is examined with respect to their capacity to inhibit of promote CO$_2$ hydrate formation.

IoLiCAP   **CO$_2$QUEST**

Gas-CCS: Experimental impact of CO₂ enhanced air on combustion characteristics and Microturbine performance

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Abstract

Due to the high certainty anthropogenic greenhouse gases, such as CO_2, have caused an increase in global temperatures threatening rising sea levels, fresh water supply, crop yields and extreme weather events, it is necessary to address the sources of emissions and mitigate them where possible.

With the present rate of GHG being released to the atmosphere it is predicted that global average temperatures could rise to almost 6C more than pre industrial levels by the turn of the century. Such a rise would be disastrous, threatening low lying cities, causing huge decline in up to 1/3 of Africa's crop yields, partial collapse of Amazonian rainforest and a much increased chance of extreme weather events, or sudden changes in key climate systems like the Atlantic thermohaline circulation. [1,2]

Globally, national strategies try to avoid picking technologies that are "winners" and "losers" but in truth the loser has already been picked due to lock in to carbonaceous fuels and the large supply. Particularly with developing economies use, retrofit of Carbon Capture & Storage (CCS) will be an essential "winner" to stay within a remaining global carbon budget to keep below a 2C rise.

This work looks to increase the efficiency of CCS post combustion capture systems. Focusing on the impact of enhancing CO_2 concentrations of inlet combustion air for a Turbec T100 micro gas turbine. The experiments are a step towards the application of exhaust gas recirculation (EGR), increasing the partial pressure of CO_2 in flue gases in order to reduce the mass flow through the absorber, and reduce the rate at which MEA solvent must be regenerated, and hence reducing reboiler duty, which is the most energy intensive step in post combustion capture.

The process of EGR is simulated through enhancement of the combustion air with CO2 to analyse some of the impact EGR may have on combustion and the turbine efficiency, as well as what improvement there will be in capture efficiency and net benefit may be expected from EGR process addition.

At the Low Carbon Combustion Centre, Beighton, the UKCCSRC has funded work under Gas FACTS to experimentally investigate the impact of EGR on a full gas turbine.

A Turbec Series 1 micro turbine has been adapted with additional instrumentation to measure pressure and temperature, and enhance the concentration by volume of CO_2 into the combustion air.
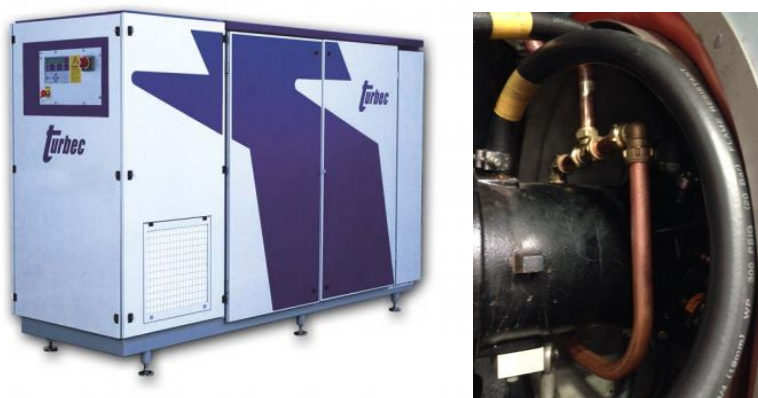
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Fig.1 T100 microturbine & copper CO2 injection line at compressor inlet [3]

The turbine has instrumentation to monitor power generated, turbine shaft speed, gas pressure, compressor inlet temperature, turbine outlet temperature, fuel inlet valve position, and pilot fuel valve position.

Exhaust gas is sampled from the turbine after CHP unit. An FTIR measures water vapor, CO_2, CO, N_2O, NO_2, SO_2, NH_3, CH4, C_2H6, C_2H_4, C_3H_8, $C_6H_{14}CHOH$, NO_x, and TOC. A Horiba VA-3000 is connected at the same point measuring the oxygen content in the exhaust.

Fuel flow is monitored, and calorific value and fuel composition is taken from regionally published data by National Grid.

A range of CO_2 enhancements representing different recirculation ratios of the gas turbine have been tested, and the collected results will be presented with comparison to the microtubines base performance, and the potential impact that may be interpreted on a large commercial Combined Cycle Gas Turbine (CCGT) power plant.

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Pressurised Carbonation Experiments in the Presence of Steam in a Spouted-Bed Reactor

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Abstract

Calcium looping is a high temperature solid looping process designed for CO_2 capture. The concept utilises the reversible reaction between calcium oxide and CO_2. The technology uses two reactors: the carbonator and the calciner. In the carbonator, a bed of calcium oxide reacts with the CO_2 to form calcium carbonate at around 650 °C. This calcium carbonate is then cycled to the calciner (operating at temperatures in excess of 900 °C) to undergo decomposition and release a pure stream of CO_2, while regenerating the calcium oxide. The calcium oxide is then cycled back into the carbonator. Previous work[1,2,3] investigating the effects of steam on the calcination and carbonation reactions has produced contrasting results. Their work either involves the use of steam in a fluidised bed at atmospheric pressures or at pressure in a TGA. The work presented here focuses on pressurised carbonation reactions in the presence of steam in a 3 kW spouted bed reactor, giving a more rigorous insight into the effects of steam at more realistic process conditions. Different experiments were carried out to determine the effects of the system pressure, partial pressure and the temperature on the carbonation reaction. Similar experiments have also been carried out in the absence of steam for comparison. The results demonstrate that the presence of steam, particularly at higher pressures, aids in both the observed rate of reaction and the conversions of the calcium oxide particles to calcium carbonate.

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Investigating the performance of Fe- based oxygen carriers for pressurised chemical-looping combustion of gaseous fuels

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Abstract

Chemical-looping combustion (CLC), typically based on circulating fluidised bed technology, is a flameless combustion technology that utilises metal oxides (oxygen carrier, OC) to transfer oxygen from air in one reactor, to the fuel in another reactor. CLC potentially offers a low cost and thermodynamically efficient way of intrinsic separation of CO_2 with very low energy penalty.

Compared to current best available technology such as natural gas combined cycle plants (NGCC), CLC for power generation with gaseous fuel would result in much lower exergetic efficiency in power generation if the fuel is not pressurised. This is because of the system is limited to a basic steam cycle (Rankine cycle), rather than a combined cycle (Brayton and Rankine cycle). The issue could be resolved, however, by pressurised the system, or by using solid fuels. Our research focuses on the performance of low-cost, iron OCs for use with natural gas or gasified solid fuels at pressurised conditions. A strong emphasis is placed on the kinetics and performance of the OC particles under pressurised conditions.

Here, we present findings from our investigations into the chemical-looping combustion of alumina-supported iron oxide (Fe_2O_3/Al_2O_3) with the main component carbon monoxide. A state-of-the-art 3 kWe lab-scale pressurised fluidised bed reactor at Imperial College, capable of operating at temperature up to 1000°C and pressure up to 20 bar, was used for simulating CLC with ex-situ gasification of solid fuels under pressurised conditions. The mechanical stability and the reduction kinetics of the particles (the rate limiting step in the CLC of gaseous fuels) over multiple cycles have been assessed at high temperatures and pressures up to 0.5 MPa. Pressurised experiments with the Fe_2O_3/Al_2O_3 shows the reaction order for the reduction with CO to Fe_3O_4 is slightly lower than 1, and a stable reactivity of the OC over repeated cycling.

Investigation of the effect of elevation and impurities on CO₂ pipeline repressurisation distance using Aspen Hysys 8.6V process simulator

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Abstract

Carbon Capture and storage (CCS) has been established as a technical credible option for the atmospheric CO_2 reduction. This is as fossil fuel continues to play a major role in the current energy mix with regards to the global energy requirement. For a long distance movement of CO_2, connecting source with a geological suitable sink, transport by pipeline remains a more economical viable option. CO_2 pipeline transport process can gather large volume of CO_2 at supercritical state and transport it effectively.

From engineering design of CO_2 pipeline flow assurance & integrity point of view, understanding adequately the effect of increase in elevation on energy requirement on the pipeline trajectory is crucial as it may result in the formation of a vapour phase which will cause the impurities to separate. The separation could triggers a whole lot of pipeline integrity issues such as corrosion, hydrate formation and blockage if water is sufficiently present and embrittlement if there is hydrogen. This work examines the points at which phase splits occur, how fast the CO_2 separated components revert to supercritical state after such an upset condition. Again, the effect of different levels of impurities on the maximum safe distance to subsequent pumping station as a function of varying topography, inlet pressure and environmental temperature is examined.

A commercially available process simulator Aspen Hysys V8.6 is used to examine a 171km conceptual CO_2 pipeline with a maximum allowable operating pressure (MAOP) of 110bar and minimum miscibility at the critical pressure with an allowance of 5bar. Various emission rates from power plant operating Combined Cyclic Gas turbine (CCGT) with 100%load, 50%,58% &60.75% efficiency and 90%,95% & 99.95% impurity content are examined. The impurities considered are SO_2, N_2, Ar, CO, Methane, H_2O, O_2 and NO_2.

The result shows that at a pressure of (85.3bar) dip (90%CO_2) from an elevation of 256m, it was not long enough (about 4km) to cause a phase split. However, when the dip in pressure is 77.2bar from an elevation of 390m and 71bar from 490m, the flow regime changes from single phase to dispersed bubble and stratified respectively indicating a vapour phase formation. On the other hand, at a constant flow rate, the pipeline distance before repressurisation for 90%, 95% and 99.95% CO_2 is longer in 99.95%CO_2 followed by 95%CO_2. This confirms the fact that the critical point of 90%CO_2 is the highest.

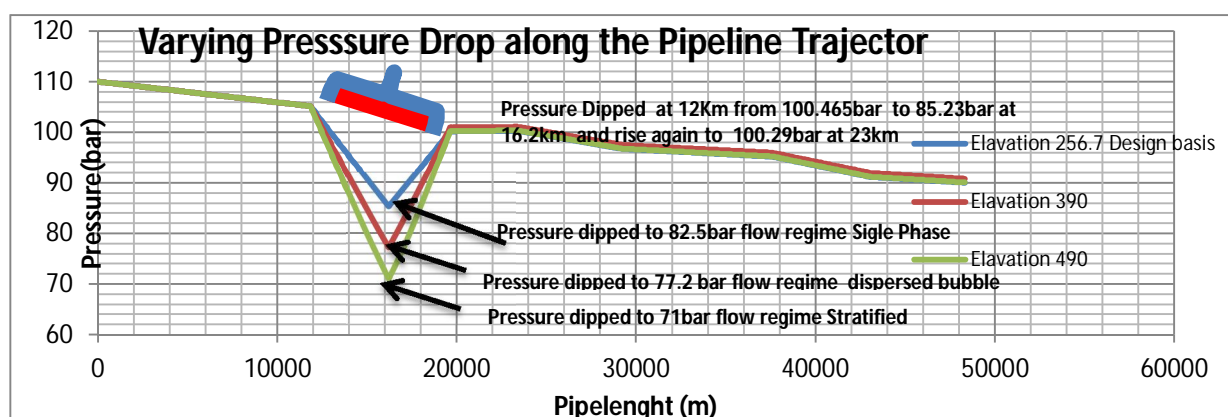Figure 1: Effect of elevation on CO2 pipeline trajectory
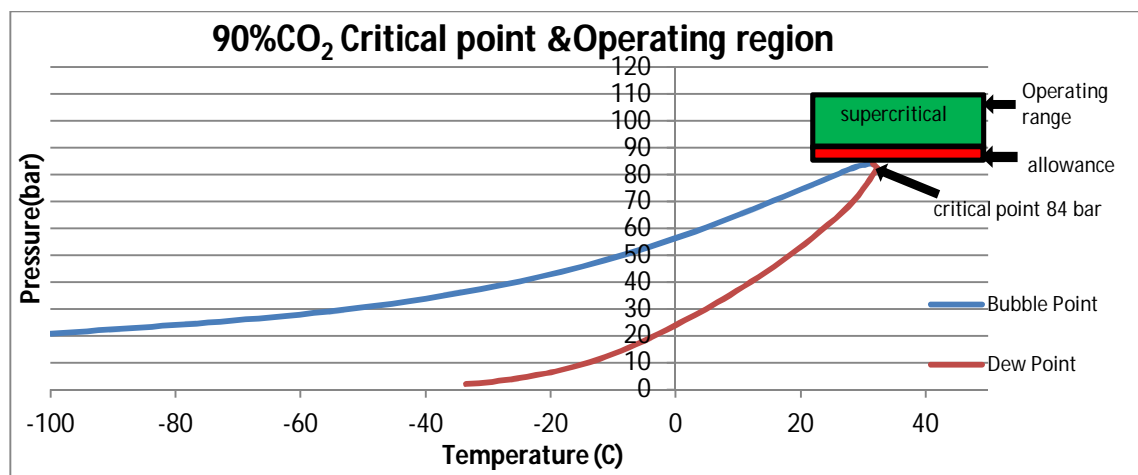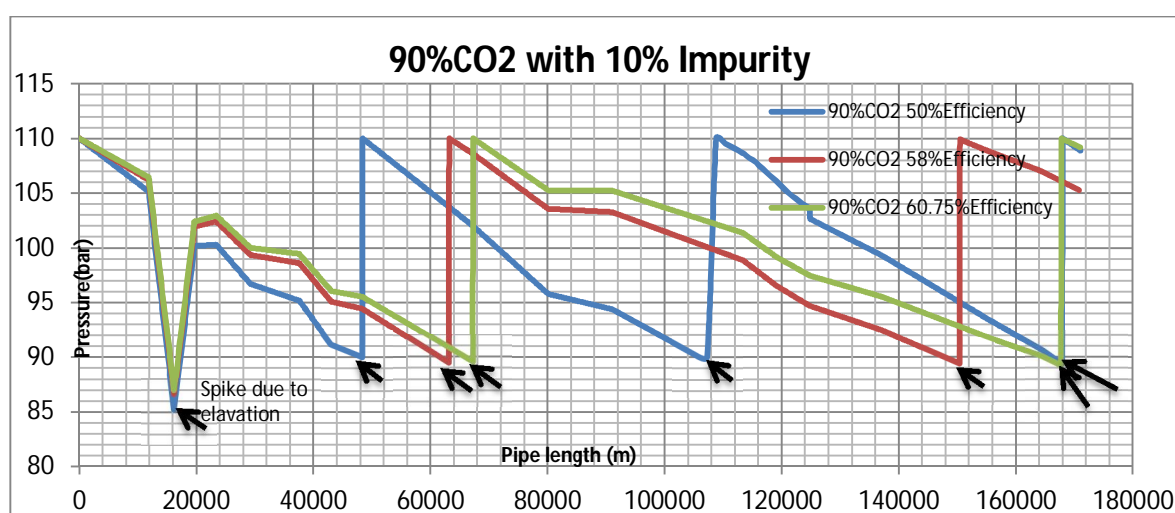
Figure 2 90%CO$_2$ Critical point

Figure 3 Effect of impurity and machine efficiency on repressurisation distance

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Feasibility Study of Microbial Associated CO2 Geological Storage

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Abstract

Among in-situ microbes within depleted oil-gas reservoir, there are special species those produce much more methane gas in CO2 rich environment than in CO2 poor environment. CO2 acts as a catalyst in the reaction. If we maintain preferable conditions for methanogenesis archaea during geological CCS, we will be able to abate greenhouse gas emission and produce natural gas as one of natural energy resources at the same time.

We named the technological concept as 'Microbial associated Geological CCS'. In Microbial associated Geological CCS, CO2 will be injected from a well for two purposes: to abate greenhouse gas emission and to cultivate methanogenic geo-microbes. CH4 gas will be produced later using other wells. The procedure is similar to the Enhanced Oil/Gas Recovery (EOR/EGR) operation, but in Microbial associated Geological CCS, the target is production of methane out of depleted oil/gas reservoir during CO2 abatement.

Based on knowledge of previous studies, we examined relationship between reactions of in-situ microbial communities and CO2 partial pressure in cultivation conditions. We collected bailed water samples those containing in-situ microbes from Yabase depleted oil-gas field in Japan. We kept containers in 55ºC, 5MPa, and measured concentrations of CO2 and CH4 partial pressures of the gas in the containers. As the result, we found specific species those accelerates CH4 production two times faster than other methanogenic species (1). The findings initiated the Microbial associated Geological CCS concept.

When we consider feasibility of Microbial associated Geological CCS technology concept, the most essential information is CH4 produce potential. To estimate production rate, we set a developed a basic geological model of Microbial associated Geological CCS process on CHEM-TOUGH simulator, and implemented microbial activities and CCS process into it. For mineralogical composition of rock matrix and formation water in depleted reservoir, we applied measured value in Nagaoka and Yabase. We assumed a fluid flow model; residual oil is a part of matrix and it will not move; fluid will flow in the rest, 0.1 real pore space. Then we obtained preliminary results of CH4 production and other masses' distributions (2).

We analyzed accident statistics of ground surface industrial facilities and oil/gas wells especially accidental leakage of CO2 and methane leak. We estimated distribution of accident probabilities and accidental leak volume for 105 ton/year CO2 injection. These accidental leak scenarios are offered for environmental impact studies and LCA analysis. As regard with risks of produced methane gas, it will vary on the quantities of the production from the well. Timescale of biological methanogenesis is different from that of CO2 injection rate. Therefore, when consider CH4 release accident, risks will be negligible other than CH4 is collected up to explosion limit (11%) of ambient air (3).

To assist basic site evaluation and help understanding of Microbial associated Geological CCS technology concept, we are preparing a prototype of Bio-CCS site evaluation system. All findings are bing integrated in to it: cultivation condition of methanogenic geo-microbes, estimation method of methane produce quantities, environmental impacts of various risk scenarios, and benefit analysis of schematic site of Microbial associated Geological CCS.

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Refining the model for numerical simulation and Bio-CCS site evaluation system, we are going to predict feasibility of Microbial associated Geological CCS technology concept. We also are going to extend applicable field of our Bio-CCS study into EOR-CCS and CCS into aquifers.

(Researches described in this poster have been carrying out as a part of 'energy resources creation by combining geo-microbes and CCS', as one of strategic research projects, AIST. It had initiated in October 2012 and will end March 2015.)

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Technical design of a CO₂ transport system from western Macedonia power stations to the Prinos oil field, Greece

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Abstract

Capture and storage of CO₂ (CCS) is a technically mature method for reducing CO₂ emissions in the atmosphere. The application of CO₂ capture technologies, especially in hydroelectric power stations, is expected to contribute significantly to the reduction of the greenhouse effect on a global scale.

In this paper we study the capture of CO₂ from power stations belonging to the Northern Network of Electrical Energy Production of the Greek Public Electricity Corporation (GPEC), in Greece. The study takes into account the transport and injection of this CO₂ into the Prinos oil field [1-3] offshore Kavala, via 3 different scenarios. These include transport firstly via coastal and underwater pipeline, secondly via trucks weighing between 20t - 40t followed by tankers and thirdly by transferring the CO₂ using offshore pipelines and tankers. The detailed scenarios are described in Table 1 below. The purpose of the study was therefore to analyse and compare different methods of transport of CO₂ and draw conclusions concerning the implementation of CO₂ transport technologies in Greece.

Scenario description	
1	Inshore and submarine pipeline
2(A)	Ship and truck rental
2(B)	Ship purchase and truck rental
2(Γ)	Ship rental and truck purchase
2(Δ)	Ship and truck purchase
3(A)	Inshore pipeline and ship rental
3(B)	Inshore pipeline and ship purchase

Table 1. Sub-scenarios for CO₂ transport

For the cost analysis we aimed to investigate the optimal choice of transport means which depends on the required amount of CO₂ to be transported, the distance between the source and the storage space, the geography and geology of the transport pathway and the existing infrastructure and transport costs. We also took into consideration the effect of the use of CO₂ for enhanced oil recovery (EOR) in transportation and storage.

The main conclusion that was made concerning the possible transport modes of the captured CO₂ is that for long journeys, transport with tankers is the more advantageous method (Figure 1.1). Firstly because it has the lowest cost per

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ton of CO_2 and secondly because it provides flexibility in case of change of CO_2 storage destination. If it is not feasible to transport by tanker, the pipeline transportation should be preferred although it does not offer the flexibility of the other modes (Figure 1.1). Truck renting is a completely unattractive solution, but their purchase and use for short investment periods is an interesting option that applies to geological storage and not in cases of enhanced oil recovery.
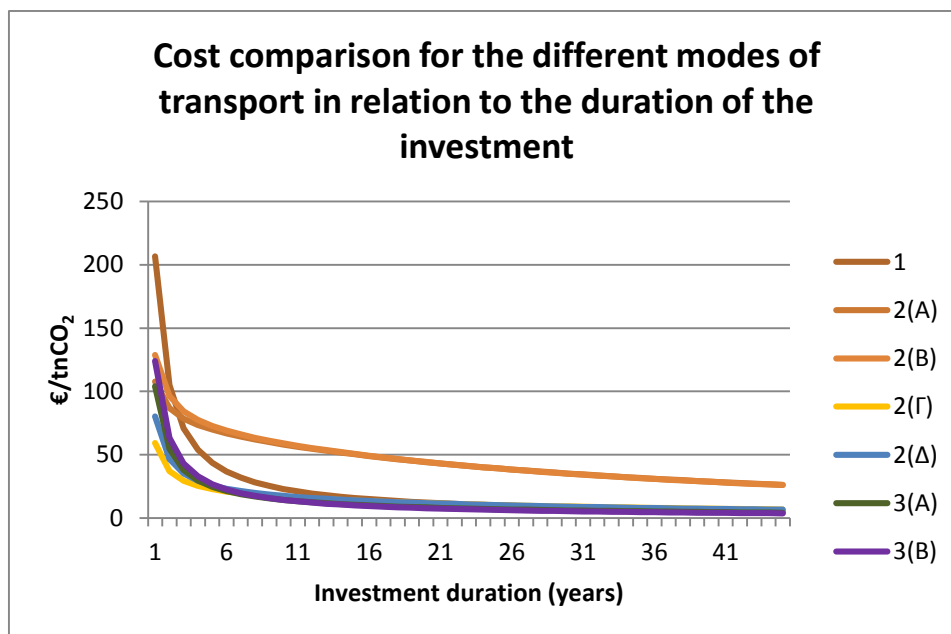

Figure 1.1 Comparison for the different modes of transport in relation to the duration of the investment

As far as the storage of CO_2 is concerned, it is known that the offshore potential reservoirs and caprocks increase the transport costs relative to other locations. However, in the case of Prinos, the additional costs are offset by the existing infrastructure located 30-40 km from the coast (pipelines, wells and platforms)[4]. Indeed, the larger the storage capacity of the formation, the more this cost can be allocated in greater amounts of CO_2 which eventually reduces the storage cost per ton of CO_2 [5].

Regarding the use of Prinos as a storage area, preliminary estimations show that the storage capacity of the existing field is not adequate for receiving the entire emissions being emitted from all the lignite power stations of the Northern System. The needs in CO_2 for "enhanced oil recovery" in Prinos are also small.

Therefore, in order to meet the needs for CO_2 storage of all the emissions from lignite power plants in the Northern system, it is proposed to make accurate estimations of the actual storage capacity of Prinos and more precisely proceed with the calculation of the possible profits resulting from enhanced oil recovery. Also an assessment of the storage capacity for CO_2 in other oil and gas fields and underlying aquifers and any other potential locations in Greece would be of interest.

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Calculation of Gas Solubility in Selected Ionic Liquids and their Aqueous Solutions with ePC-SAFT

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Abstract

The electrolyte PC-SAFT (ePC-SAFT) [1,2] equation of state (EoS) was chosen as the most reliable model for systems with ionic liquids (ILs). This is due to the electrostatic interactions that are accounted for explicitly in ePC-SAFT. The thermodynamic toolkit of the MAPS platform of Scienomics, namely SciTherm, was extended to include the ePC-SAFT model.

Some of the ILs studied were the imidazolium-based ($C_n$mim, n=2, 4, 6, 8) ILs with the anions Tf_2N and TCM. Experimental data for Tf_2N and TCM were taken from the literature and other groups of the IOLICAP project. The ILs were modeled as pseudo-binary mixtures of cations and anions. The ions were parameterized by fitting, simultaneously, against density data of different pure ILs containing these ions.

The solubility of CO_2 in the above-mentioned ILs was calculated and compared with experimental data [3]. An example is given in Figure 1 where P-T isopleths of CO_2 solubility in [C_4mim][TCM] are shown for different CO_2 mole fractions. Pure predictions with no adjustable parameters (k_{ij}=0) are shown with the solid lines. As can be seen ePC-SAFT is a reliable model even without adjustable parameters. The error can be further decreased by using one parameter (k_{ij}) fitted on one isopleth (here the x_{CO2}=0.1). The fitted kij is used for calculating the other isopleths. The results are shown with the dashed lines. As can be seen in Figure 1, calculations outside the fitting regime are in good agreement with the experiments.
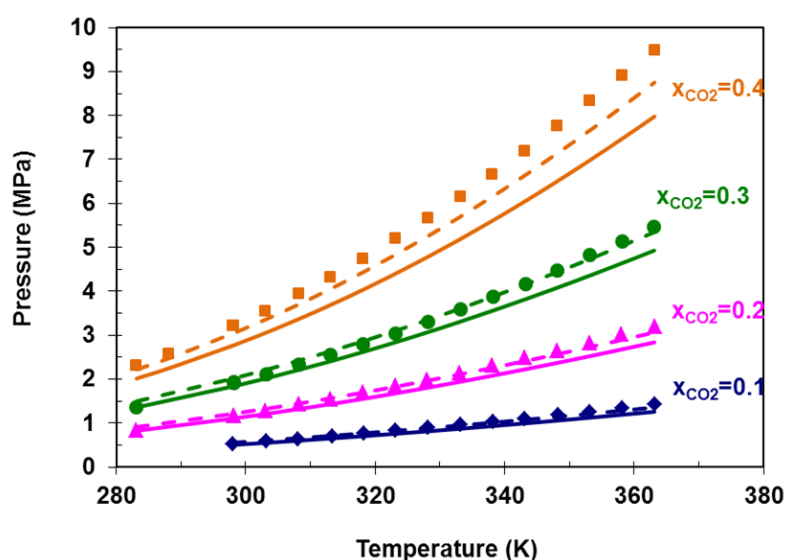
Figure 1. P-T isopleths of CO_2 solubility in [C_4mim][TCM] at different CO_2 mole fractions calculated with k_{ij}=0 (solid lines) and kij fitted to x_{CO2}=0.1 (dashed lines).

The solubility of other gases such as N_2, SO_2, C_3H_6 was calculated and found in good agreement with experimental data [4]. The good agreement between ePC-SAFT and experimental data for other gases as well as CO_2 even without adjustable parameters is very encouraging for the use of this theoretical tool for calculating solubility of various gases in ILs.

The effect of water on the solubility of CO_2 in ILs is important from an application point of view. However, limited data are available for comparison with the ePC-SAFT. We examined first ternary systems like $[C_4mim][PF_6]/CO_2/H_2O$ and $[C_4mim][BF_4]/CO_2/H_2O$ for which experimental data were available in the literature. Subsequently, we examined other anions which are of interest to this project. In some cases, the EoS predicted trends of CO_2 solubility as a function of water concentration were different from the experimental observations [4]. To interpret these discrepancies the excess molar volume was calculated and compared with experimental data. Also the effect of the water model and the relative permittivity were explored.

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4.   IOLICAP partner NCSRD MESL Dr. G. Romanos.

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Multi-Criteria Decision Support for Evaluating CCS Technologies

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Abstract

Despite the fact that CCS is being acknowledged as a key technology for achieving the EU carbon reduction targets [1] and mitigating climate change [2], there is still a lack of public acceptance. This is partly due to limited understanding associated with the technologies involved and the perceived risk and uncertainty. Therefore, there is a need to prove the sustainability of CCS over the whole supply chain by considering not only economic, but also environmental and social criteria. Moreover, challenges of limited models and data availability need to be addressed systematically. This will facilitate better informed decision making for choosing the most sustainable options and present this in a clear way that can be communicated to the general public.

The goal of this industry-focussed research is to address the given challenges in a rational way. For this purpose, a Multi-Criteria Decision Analysis (MCDA) framework that incorporates sustainability criteria over the whole life cycle has been developed. This includes life cycle costing (LCC), life cycle assessment (LCA) and other context specific measures. Major emphasis is given to stakeholder participation to enable a holistic perspective and higher confidence in the results. In order to facilitate communication, numerical results are visualised. Contributions and scoring of the chosen criteria are depicted which help to identify most relevant parameters. Moreover, risk and uncertainty are considered explicitly to be able to determine not only numerical results, but also evaluate the confidence that can be attached to the estimated values. The framework follows the steps depicted in figure 1:
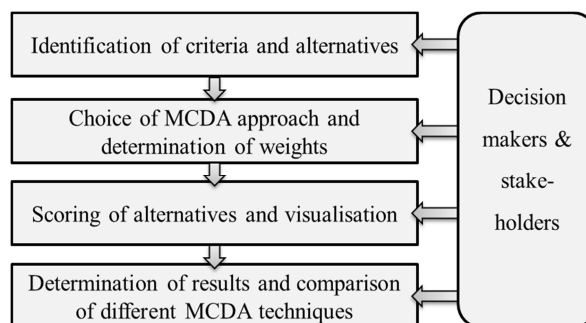
Figure 1. MCDA framework

The framework is currently applied in the shipping sector for evaluating the different material choices (HSLA and composites) to replace conventional steel components in the ship structure [3]. A life cycle cost assessment combines economic, environmental and risk factors to determine quantitative performance measures and thereupon identify optimum solution. The whole evaluation is done in close cooperation with the stakeholders involved. Numerical results are visualised with the aid of spider chart diagrams as depicted in figure 2. They help to visualise performance on different measures, such as technical, economic, environmental or social criteria. Weights can be applied to prioritise between them.
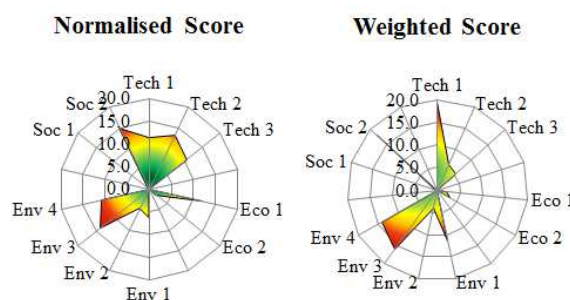
Figure 2. Visualisation of normalised and weighted scores for evaluating one alternative

Alongside refinement of the framework, it is being targeted towards application in the CCS field. It offers a suitable approach for evaluating CCS technologies, notably given that economics alone will often not provide sufficient justification for CCS implementation. Moreover, risk and uncertainty are considered explicitly, involving stakeholders throughout the process. The confidence attached to numerical results can be calculated and visualised. In this way it is possible to understand, reduce and communicate risks in a clear way which helps to address not only technical issues, but also public perception. Together, these features shall support decision making in the CCS field. A suitable case study is currently under consideration.

The approach provides considerable innovation in decision support for evaluating CCS technologies, considering the whole life cycle. It will help to deliver a holistic problem understanding and thus support informed decision making. This can be achieved through the consideration of a holistic set of sustainability criteria whilst explicitly incorporating risk and uncertainty. In this way the approach adds value to the decision making process and enables CCS practitioners to demonstrate the systematic integration of sustainability aspects to their stakeholders. Thus it facilitates to overcome not only technical barriers, but also helps to address public perception and increase confidence in CCS.

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Effect of Cryogenic Air Separation Purity on Oxy-fuel Combustion for Carbon Capture

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Abstract

Oxy-fuel combustion[1] has been widely identified amongst the most promising technologies for carbon capture and for achieving significant reductions in greenhouse gas emissions in a cost effective manner. By replacing air with nearly pure oxygen, the combustion is carried out in conditions that result in a flue gas stream rich in carbon dioxide that can easily be further purified before being sent to compression and sequestration. A simplified flow diagram of a coal-fired oxy-fuel combustion carbon capture plant is shown in Figure 1.
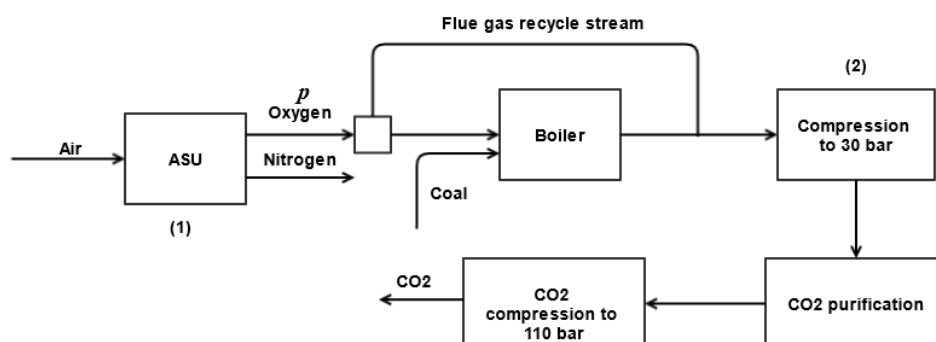
Figure 1 – Simplified flow diagram of an oxy-fuel combustion carbon capture plant.

The cost of producing high purity oxygen on-site in the cryogenic air separation unit (1) is the major contributor to the CO_2 avoidance costs of oxy-fuel combustion due to its high energy requirements, despite recent efficiency improvements[2].

Within the scope of this work, we study how the purity of produced oxygen, p, affects the energy consumption in the air separation unit (1), and in the flue gas compression train (2). We here assume that the CO_2 from the purification step operates at a fixed specification, and therefore the purity p has no effect on the energy consumption in the final CO_2 compression train.

To study the effect of producing oxygen with different levels of purity in the processes (1) and (2), these are modelled in Aspen Plus. The cryogenic air separation unit modelled in Aspen Plus is a typical two-column distillation process, as shown in Figure 2.
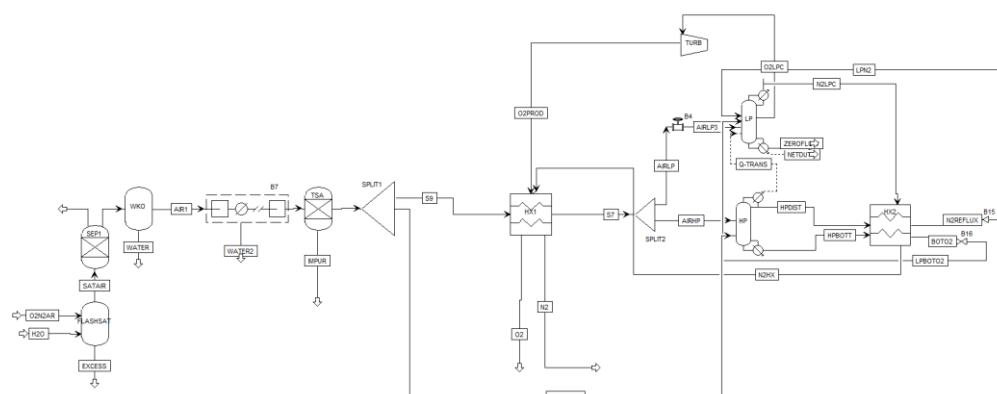
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Figure 2 – Flowsheet of the cryogenic air separation unit implemented in Aspen Plus.

Air enters the process with a flow rate determined by the amount of oxygen inlet required to produce 10,000 ton of purified oxygen per day[3]; this target corresponds to the typical oxygen needs of an oxy-fuel combustion carbon capture plant. The air separation takes place in a double-column cryogen distillation system, where oxygen is produced at the required purity. For this work, the process conditions are adjusted in order to produce oxygen with a purity in the range of 80%-99%.

The main results of this work are the energy consumption profiles for different oxygen purity levels in the cryogenic air separation unit and downstream CO_2 compression train, shown in Figure 3.
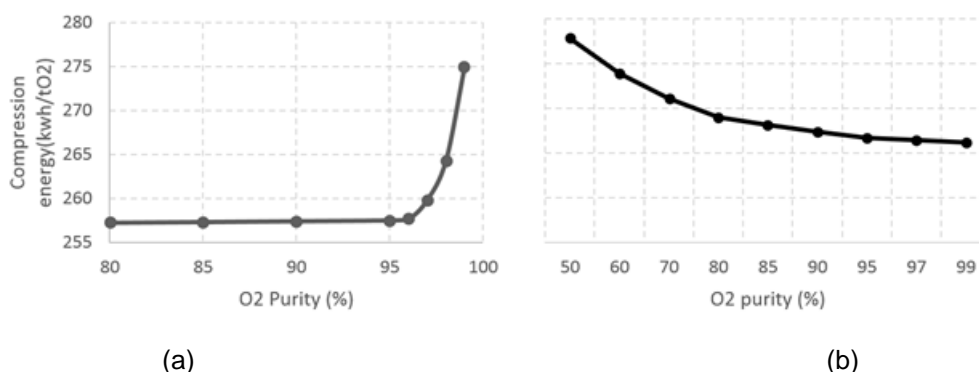

(a)   (b)

Figure 3 – Energy consumption for different oxygen purity targets in: (a) cryogenic air separation unit (b) CO_2 compression train.

As shown in Figure 3, the oxygen purity has an opposite effect in the cryogenic air separation unit and in the compression train; this trade-off is discussed in the presentation. Additionally, we outline future work directions towards the study of the effect of impurities on the entire oxy-fuel combustion carbon capture plant.

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A model of the near-field expansion of CO2 jet released from a ruptured pipeline

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Abstract

The accidental release of high-pressure sub-cooled liquids from pipes or tanks results in metastable high speed under-expanded jets, creating shock waves and inducing phase change in the region close to the release plane [1, 2]. Due to their complex non-equilibrium multiphase structure, the modelling of such jets is commonly performed either using simple heuristic and semi-analytic zero-dimensional models of the expansion flow [3], which have been shown to have low accuracy, or using highly-sophisticated computational fluid dynamic models which are inherently extremely time consuming [1, 4]. In this work, several available analytical models are analysed and compared; those are, shock fitting method, integral method based on conservation equations and evaporation wave method based on Chapman–Jouguet condition [5, 6]. A robust analytical quasi-one-dimensional model is developed with the capability of predicting initial degree of superheating and subsequent homogenous equilibrium flow of a flashing fluid. By application of a rigorous equation of state to describe fluid properties, entropy increase due to shock formation and non-equilibrium behaviour during jet expansion are captured. In addition, the importance of turbulent and viscous interactions with the free boundary is investigated. The resultant algebraic system is shown to provide a more accurate, yet computationally efficient solution, as compared to other models suggested previously. The model is then applied to study a hypothetical scenario of CO_2 release from a ruptured CO_2 pipeline.

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Compression Requirements for Post-Combustion, Pre-Combustion and Oxy-Fuel CO_2 Streams in CCS

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Abstract

The efficacy of Carbon Capture and Sequestration (CCS) as a means to mitigate the CO_2 gas emissions from industrial sectors requires the minimisation of the costs associated with compression and transportation of CO_2 streams carrying various amounts of impurities. In the present study, a thermodynamic analysis method is applied to determine the power requirements for compression of captured CO_2 gas to a dense-phase liquid at 151 bar pressure for the pipeline transportation and geological storage. The study examines several compression options, which employ conventional 8-stage integrally-geared centrifugal compressors (option A), advanced supersonic shockwave 2-stage compressors (option B), 5-stage centrifugal compressors combined with subcritical liquefaction and pumping unit (option C) and 7-stage centrifugal compressors combined with supercritical liquefaction and pumping (option D) [1, 2]. The study is performed for typical conditions of operation of a coal-burning 900 MW power plant with the CO_2 emissions of *ca.* 156.4 kg/s, where the CO_2 streams captured in post-combustion, pre-combustion and oxy-fuel, are assumed to have purity of 99.664, 98.066 and 81.344 % v/v, respectively as shown in Table 1.

	Oxy-fuel	Pre-combustion	Post-combustion
CO_2(% v/v)	81.344	98.066	99.664
N_2(% v/v)	8.5	0.02	0.29
O_2(% v/v)	6.0	-	0.0035
Ar(% v/v)	4.0	0.018	0.0210
SO_2(ppmv)	800	700	67.10
NO_2 (ppmv)	609	-	38.80
H_2O (ppmv)	100	150	100
CO (ppmv	50	1300	10
H_2S (ppmv)	-	1700	-
H_2 (ppmv)	-	15000	-
CH_4 (ppmv)	-	110	-

Table 1.   Compositions of CO_2 mixtures captured from oxy-fuel, pre- and post-combustion technologies, adopted in the present study [3].

The study accounts for the different pressures and temperatures of CO_2 streams captured using the above three technologies, which were set to 1.51 bar, 38 ^{o}C for post-combustion [1, 4], 35 bar, 25 ^{o}C for pre-combustion [5] and 20 bar, 18 ^{o}C for oxy-fuel [6] captures. The compression power is calculated assuming realistic efficiencies of the compressors, pumps and intercooling units by applying the Peng-Robinson equation of state (PR EoS) to predict the thermodynamic properties of the CO_2 mixtures.

Figure 1 shows the total power consumed for compression of the various CO_2 streams and operating inter-stage water cooling pumps in the multistage compression options A, B, C and D. As can be seen from Figure 1, for post-combustion and pre-combustion CO_2 streams, option C can potentially offer higher efficiency than conventional 8-stage compression (option A).
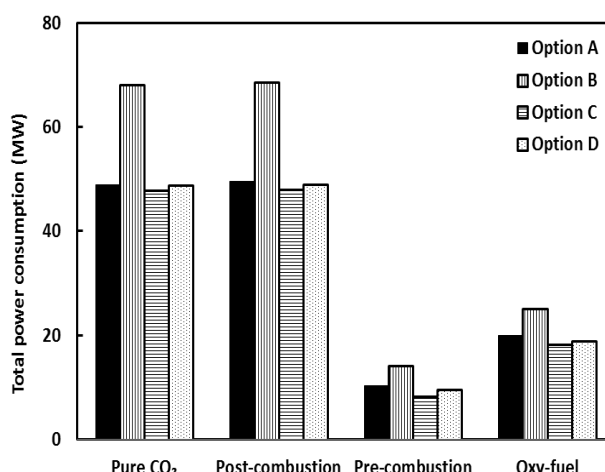
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Figure 1. Power consumed in terms of compression and inter-stage cooling of multistage compression options A, B, C and D for the various CO_2 streams.
Option A: 8-stage integrally centrifugal compressor.
Option B: 2-stage advanced supersonic shockwave compressor.
Option C: 5-stage compression combined with subcritical liquefaction and pumping.
Option D: 7-stage compression combined with supercritical liquefaction and pumping.

In case of oxy-fuel mixture, which carries relatively large amount of impurities and has significantly lower boiling temperatures than pure CO_2, the option C proved to be less feasible due to the requirement of cryogenic temperatures for liquefaction purpose, while option D efficiency is only marginally lower than that in the option A.

Implications of the results of the thermodynamic analysis for the design/operation of compressors of CO_2 streams of various purities, and the overall costs of CO_2 capture, purification and transportation are discussed.

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Comparison of numerical predictions with CO_2 pipeline release datasets of relevance to CCS applications

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Abstract

Carbon capture and storage (CCS) refers to a set of technologies designed to reduce carbon dioxide (CO_2) emissions from large point sources of emission such as coal-fired power stations, in order mitigate greenhouse gas production. CCS technology, or sequestration, involves capturing CO_2 and then storing it in a reservoir, instead of allowing its release to the atmosphere, where it contributes to climate change. Necessary transportation can be achieved in different ways, but it is commonly acknowledged that high pressure pipelines transporting liquid CO_2 will be the most reliable and cost effective choice. Their safe operation is of paramount importance as the inventory would likely be several thousand tonnes and CO_2 poses a number of dangers upon release due to its physical properties; it is a colourless, odourless asphyxiant which sinks in air and has a tendency to solid formation upon release with subsequent sublimation. It is directly toxic in inhaled air at concentrations around 5% and likely to be fatal at concentrations around 10%.

A number of projects have included experiments investigating the behaviour of high pressure CO_2 releases simulating accidental or operational CCS scenarios. Typically these are dense phase pure CO_2 releases into air with varying levels of humidity. Data is available in the public domain, either published or freely downloadable, from the CO2PIPETRANS, CO2PIPEHAZ and CO2QUEST European-funded projects, from the industry-funded COOLTRANS research programme and from laboratory scale experiments e.g. [1].

In this paper, we perform the first overall comparison between the available datasets by employing our state-of-the-art multi-phase heterogeneous discharge and dispersion model. This model is capable of predicting both near and far-field fluid dynamic and phase phenomena and has been validated against a number of datasets for free releases [2,3], punctures of buried pipelines [4] and ruptures of buried pipelines [5,6]. Predictions are based on the solutions of the ensemble-averaged, density-weighted forms of the transport equations for mass, momentum, and total energy. A comparison is also provided between achieving closure of this equation set with a compressibility-corrected k-turbulence model and a compressibility-corrected Reynolds-stress turbulence model with novel coefficients validated against air-jet releases. Finally, we also compare numerical predictions produced from different equations of state (EoS), including predictions obtained with our original composite EoS [7](consisting of Peng-Robinson [8] in the gas phase, Span and Wagner [9] in the liquid phase and DIPPR in the solid phase), with the use of the Jager and Span EoS for solid phase CO_2 [10] instead, and with molecular SAFT-based models, producing the first comparison of available EoS for modelling CO_2 releases in CCS scenarios.

The results of these comparisons will inform far-field modelling of CO_2 release scenarios and entire chain CCS quantified risk analysis, benefitting academic, industry and regulatory stakeholders.

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Industrial scale CO2 release experiment facility modelling CO2 pipeline failure

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Abstract

The facility of full instrumented industrial scale CO2 pipeline used for modeling CO2 leakage, which was funded by EU in the projects of CO2PipeHaz and CO2QUEST, has been relocated in Anbo town, Dalian city in China. Figure 1 shows the scheme diagram of the CO2 pipeline as well as the photos of the real pipeline.
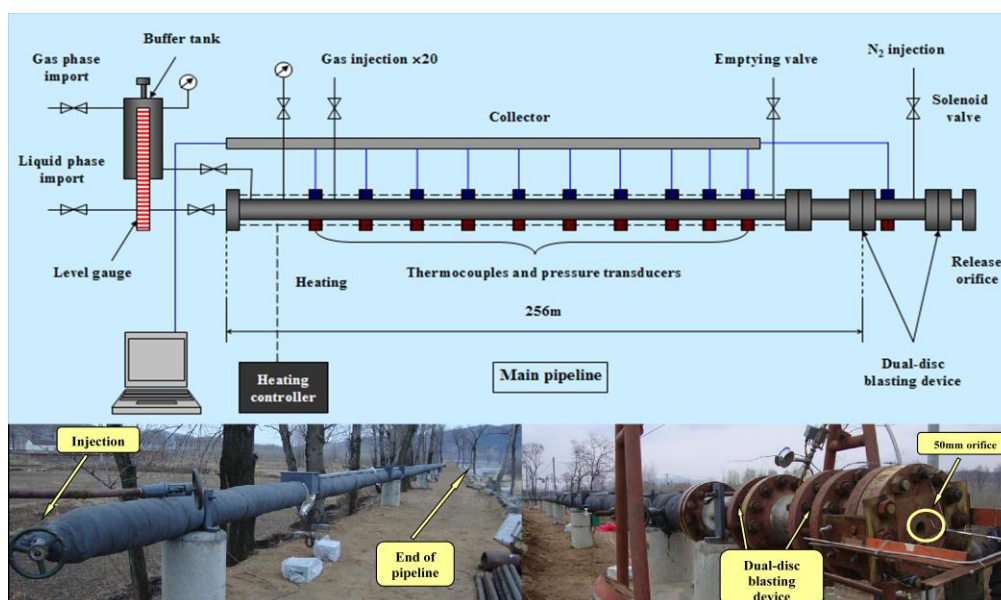
Figure 1. The full instrumented 256 m long CO2 pipeline in Anbo of Dalian in China.

This 256 m long, 20 mm thickness carbon steel pipeline had been used to perform all kinds of CO2 release experiments including supercritical CO2 (as high as 86 bar), gas-liquid and gaseous releases and generated a large amount of data both for the fluent in the pipeline and in the dispersion area. Our cooperated paper had been published [1, 2] and explained the data using related models.
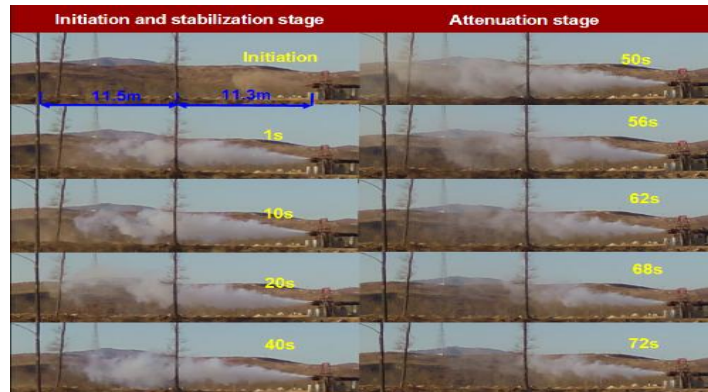
Figure 2. CO2 release using the industrial scale pipeline.

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Synthesis of selective CO_2 sorbents for post-combustion capture: The key role of the intrinsic basicity originated from oak wood

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Abstract

Selective CO_2 sorbents were successfully synthesized through the physical (CO_2) activation of oak wood-based chars. Raw material was previously carbonized either by pyrolysis at 800 °C and by hydrothermal synthesis (HTC) at 250 °C. A more dramatic development of texture was attained for the hydrothermally carbonized biomass, therefore promoting HTC as a cost-effective route for the preparation of porous activated carbons (ACs). ACs thus synthesized along with a commercial carbon included for comparison purposes were tested for CO_2 capture by using a thermogravimetric analyser (TGA). Under pure CO_2 and 35 °C, although having much lower surface areas (highest S_{BET} = 627 m^2/g), oak wood-derived carbons exhibited uptakes as large as those achieved by the commercial AC (S_{BET} = 1231 m^2/g). This finding was attributed to the comparable ultramicropore volume (d<0.7 nm) measured for all the samples. This suggests that carbon dioxide is mostly adsorbed onto the narrowest pores. On the other hand, upon changing to post-combustion conditions (ca. 53 °C, 15 % CO_2/85 % N_2), oak wood-based sorbents exhibited similar (OW250PA) or even greater (OW800PA) sorption capacity than the commercial AC. The higher selectivity shown by oak wood derivatives was associated with their substantial amount of Ca-based inorganic fraction. This was revealed by EDX and was evidently related to the outstanding basicity measured by Boehm's titrations on the synthesized sorbents' surface (up to 93 %). Conversely, commercial AC is characterised by a far poorer inorganic content, thus showing lower basicity (ca. 67 %). Accordingly, it was proved that under post-combustion conditions the contribution of a more favoured (basic) surface chemistry outweighs the texture effect. Basic functionalities ensured stronger interactions with the carbon dioxide molecule, therefore implying a more selective sorption at lower gas concentration. Therefore, it was demonstrated how selective CO_2 sorbents could be prepared exploiting the advantageous properties of the raw biomass rather than applying expensive and environmentally unsustainable chemical treatments.
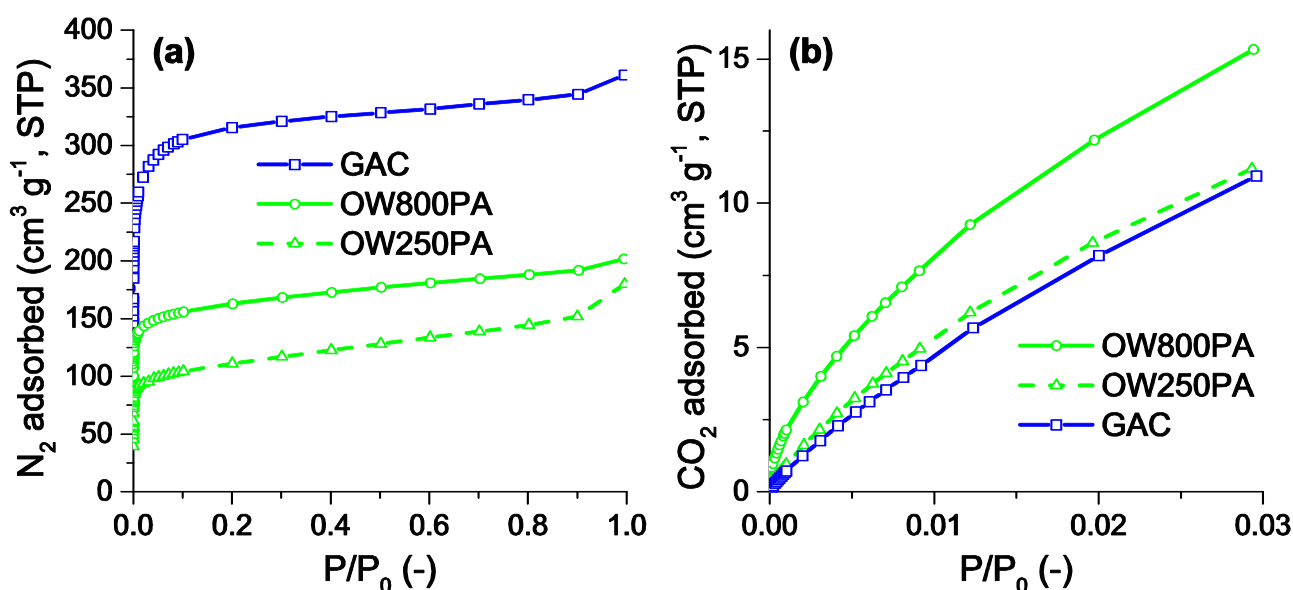
Figure 1. N_2 (a) and CO_2 (b) adsorption isotherms for oak wood-derived and commercial carbons
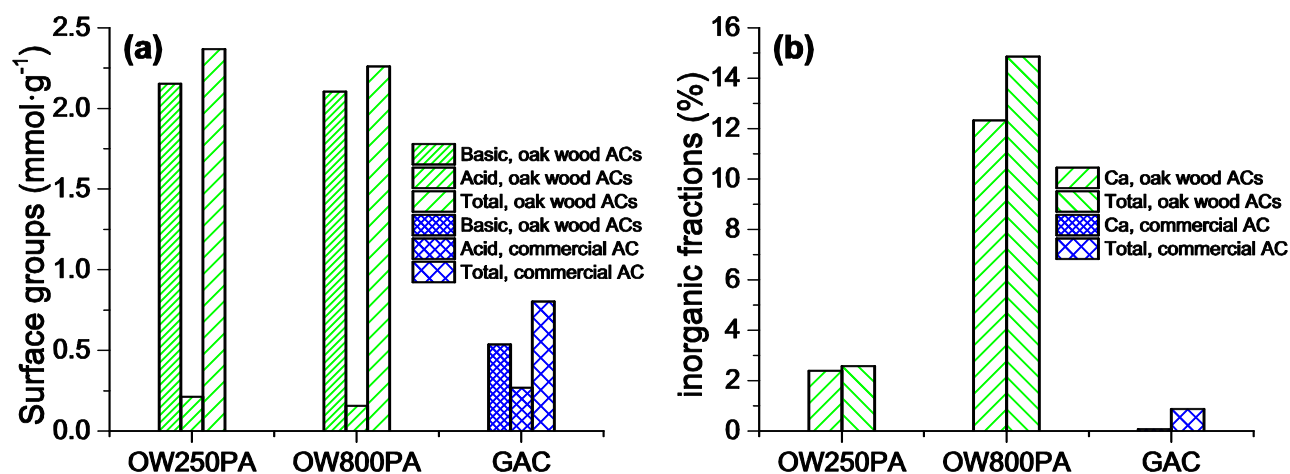
Figure 2. Surface groups number (a) and inorganic content (b) for oak wood-derived and commercial carbons
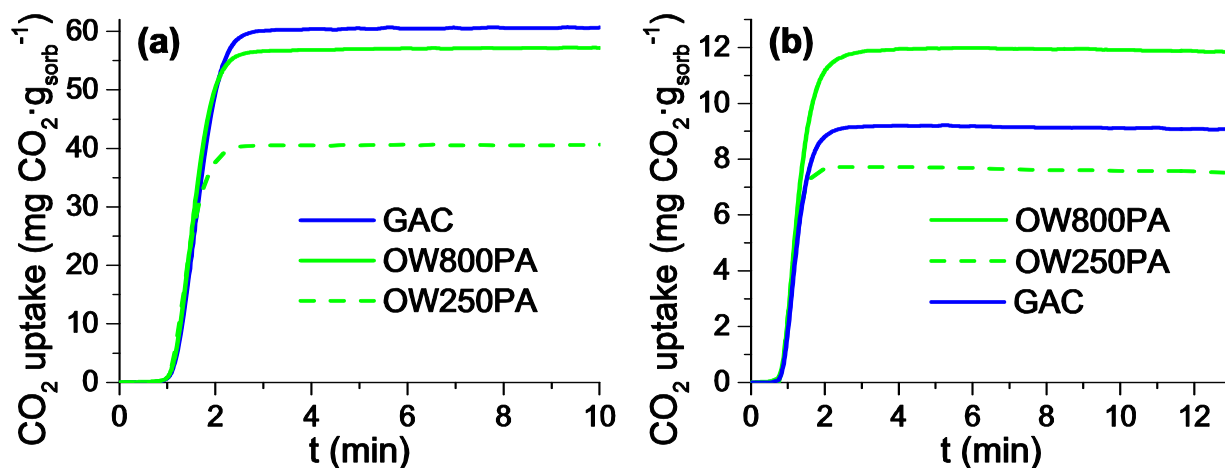

Figure 3. CO_2 uptakes measurements for oak wood-derived and commercial carbons: pure CO_2 and 35 °C (a), and 15% CO_2 and 53 °C (b)

Sample ID	CO2 uptakes, TGA		N2 and CO2 adsorption isotherms			Boehm's titrations		EDX	
	Pure CO_2, 35 °C ($mgCO_2/gs_{orb}$)	15% CO_2, 53 °C ($mgCO_2/g_{sorb}$)	S_{BET} (m^2/g)	V_{mi} (cm^3/g)	V_{umi} (cm^3/g)	Basic surface groups (mmol/g)	Basic/Total (%)	Ca (wt. %)	Total (wt.%)
GAC[1]	60.6	9.0	1231	0.474	0.026	0.54	67	0.08	0.88
OW800PA[2]	57.1	11.8	627	0.240	0.040	2.11	93	12.32	14.86
OW250PA[3]	40.6	7.2	415	0.173	0.028	2.15	91	2.39	2.58

Table 1. CO_2 Uptakes, textural parameters and basicity for oak wood-derived and commercial carbons

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[1] Commercial carbon.
[2] Oak wood, pyrolysed at 800 °C, physically activated.
[3] Oak wood, hydrothermally carbonized at 250 °C, physically activated.

Inside and outside flow from pipes containing a dense CO2 mixture incorporating impurities: experimental set-up and first results

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Abstract

Within the frame of the European project CO2Quest [1,2], medium-scale experiments are underway involving high pressure releases of CO2 containing a range of impurities such as those potentially left from a capturing operation. A dedicated experimental rig was developed so as to investigate the influence of those impurities on the flow inside and outside the pipe. The setup (Figure 1) includes a 37.5 m long 50 mm i.d. pipeline equipped with several sets of pressure and temperature transducers placed along the tube each12 meters. Outside, the "expansion zone" of the jet is specifically instrumented with pressure transducers and thermocouples. The pipe is insulated, and equipped with a mixing system. The latter is basically a pump recirculating the mixture and the impurities are injected in the loop. The mixture is pumped at one end and reinjected at several locations. The composition of the mixture is controlled by sampling and gas chromatography. The chosen impurities are nitrogen and methane and were compressed and inside a bottle and connected in series on the loop. The pipe is supported by 6 masts equipped with electronic weighing devices so as to measure the leakage mass flowrate. A calibrated orifice is placed at one end to allow some variations of this flowrate. A transparent section is provided at mid-length to follow the evolution of the flow (liquid, two phase,..). Films were made.

Figure 1: Left: Weighing masts (blue) with pipe; center: global view of the pipe; Right: near field equipment

Almost 30 tests were run, varying orifice diameters, initial conditions and mixtures. The experimental conditions of three typical tests are presented on the table below:

orifice diameter	Pressure	Ambient temperature	Mixture	Liquid analysis (before release)	gas analysis (after)
12 mm	65 bar	25 °C	pure CO2 (liq)	-	-
6 mm	63 bar	18 °C	CO2 + 4.5% CH4	CO2 + 4% CH4	CO2 + 0% CH4
6 mm	65 bar	13°C	CO2 + 4.5 % N2	CO2 + 3.5 % N2	CO2 + 0% N2

Table 1: Experimental conditions

The evolution of the mass versus time, at each measurement point, coupled with the knowledge of pressure and temperatures inside the pipe, permits to plot the evolution of the normalised liquid level in the pipe (h/D). It is also possible to plot the evolution of the mass flow rate versus time. Two ways of calculation are chosen, the first one (red line on figure 2-right) concerns a temporal derivation of the mass released, the second one is calculated using the derivation of the polynomial representing the first 20 seconds of the mass released. The first period (a few hundred of milliseconds after the start of release) corresponds to the short period of time where the fluid inside the pipe is nucleating but seems homogenous. The next period (3 s) corresponds to the period where a defined two phase mixture is present in the pipe and the level of liquid is above the orifice location. At this point, the level of liquid reaches the orifice. After 8 s, the level of liquid is below the orifice line. The two-phase flow ends after about 20 s when there is only vaporised CO2 left in the pipe.
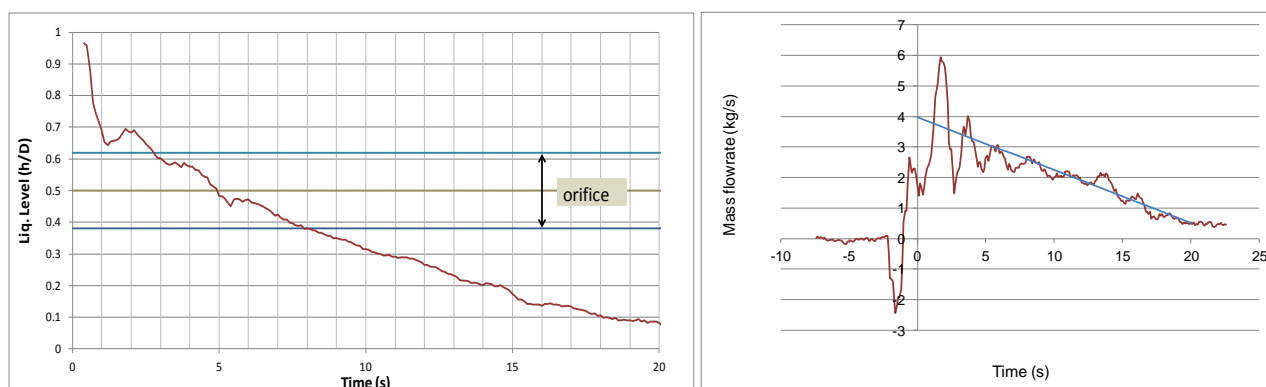

Figure 2: Liquid level and mass flow rate evolution versus time

At each of the four measurements points, 4 thermocouples (3 inside and 1 on the skin), two flux meters, and a pressure probe are installed. In figure 3, the evolution of the pressure close to the release point is plotted as function of the temperature for the three internal thermocouples for two mixtures, CO2+4.5% CH4 (left) and CO2+4.5% N2 (right). It can be seen the points lying below the saturation line in the gas phase domain.
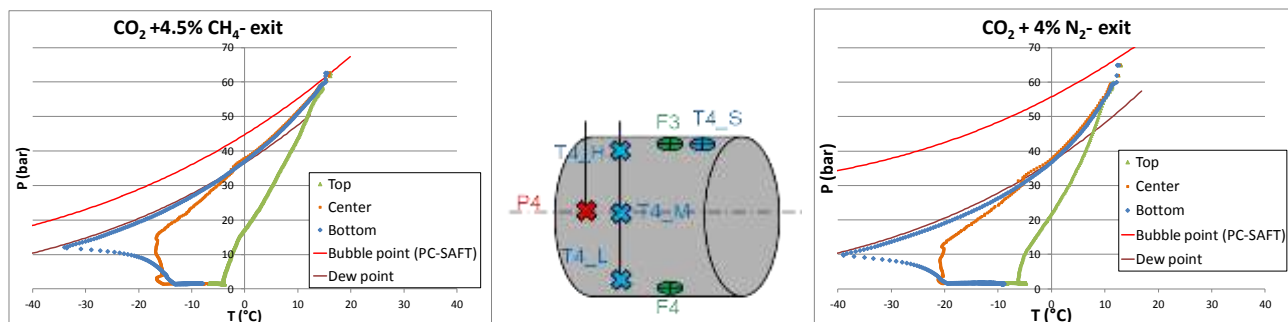

Figure 3: Temperature evolution inside the pipe as function of time

The comparison with bubble curves obtained with simulations (PC-SAFT) seems showing, for both mixtures, stratification. The gas impurities concentrations are higher on the surface layers. A gas chromatography analysis near the filling connection just before and after the blowdown test confirms the non homogeneity of the mixture (see table 1). Before the release, the concentration values are closed to those anticipated, and after the release, the gas analysis reaches zero percent of impurities.

References

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CO₂ and its impurities along the CCS chain : overview of possible impacts and criteria for risk assessment

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Abstract

One objective of the CO2Quest project is to design a risk assessment and environmental analysis methodology, based on combination of the different effects of impurities. Therefore we aim to incorporate safety and impact aspects in decision making tools.

The first basis for such a work is the overall methodology that was already described by INERIS for the whole CCS chain [1]. The objective is to define an adequate workflow for risk assessment, that includes practices from industrial safety and from underground risk management. It appears that all risk scenarios, either sudden or long-term, have the general pattern that is described on Fig.1:
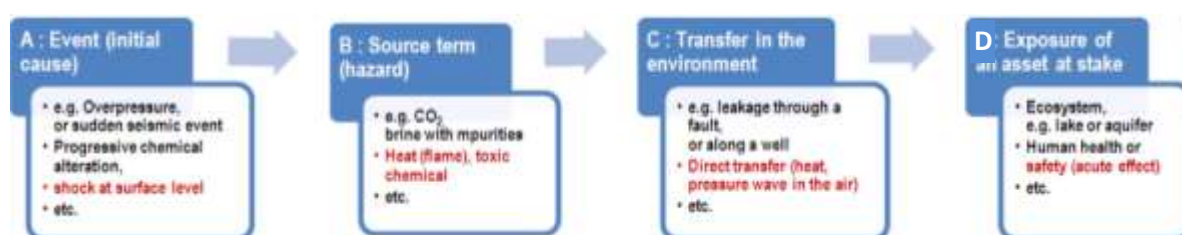

Figure 1: Graph describing risk scenarios - in red colour: sudden events, generally linked to industrial equipment [2]

This pathway from the initial event (A) to the final exposure (D) was described in Farret, 2001 [2]. Regarding exposure (D), generic categories of 8 "impacting phenomena" were also defined (e.g. fire, pollution, mechanical effects, etc.)

The second basis is an overview of the current knowledge about annex substances in the CO_2 stream. They are (i) "major" annex gases such as O_2 or Argon, (ii) gases present in lesser quantities such as H_2S or NO_2, or (iii) toxic impurities such as metals or organics. INERIS and partners explained the undesirable effects of these annex substances. For each impurity, 3 categories of impacts are identified:

- the physical impacts,
- the chemical impacts,
- the toxical and ecotoxical impacts.

As concerns toxicity, a review of all impurities was performed in order to identify the possible effects, either in case of an accidental release, or for longer term (e.g. in case of a leakage from a storage to an overlying aquifer).

As concerns the physical impacts, they concern only annex gases but they cover both transport and storage. Well-known effects are the modification of physical parameters, such as density, viscosity, compressibility – These effects will impact the transport stage (see higher part of Fig.2) but may also influence the storage capacity because a lower density gives a lower storage capacity, a lower lateral spreading or a lower residual trapping (see lower part of Fig.2). The solubility trapping may also be reduced, due to a lower solubility in water.
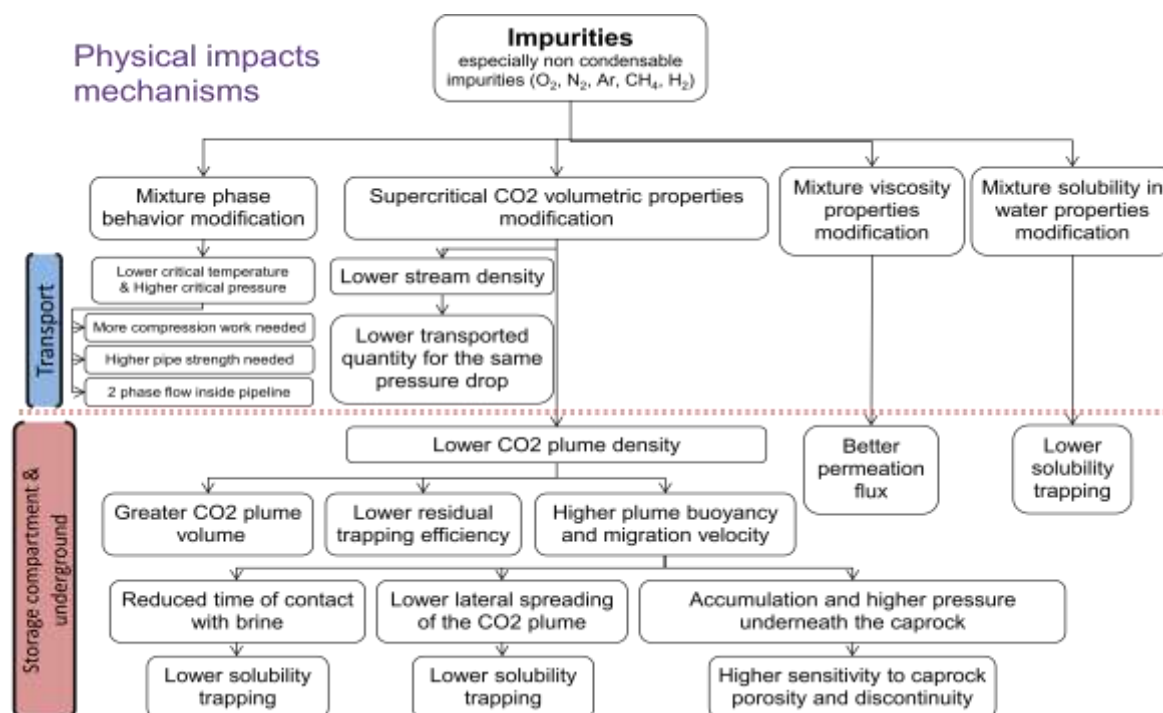
Figure 2: Grah presenting the physical impacts of impurities in the CO_2 (higher part: transport, lower part: storage)

Then, we defined parameters -such as "higher buoyancy", "pore plugging", etc.- that reflect all potential impacts and that can be quantified with a scoring scale. For each annex substance, a global matrix tool describes these parameters, the induced impacts and the limit whenever identified (e.g. toxicity thresholds, limit for plume density).

For a given CO_2 stream composition with a number of given annex substances, the objective is to provide a global representation of the impact of impurities along the CCS chain by aggregating the scores gathered for the parameters identified. Fig.3 gives an example.
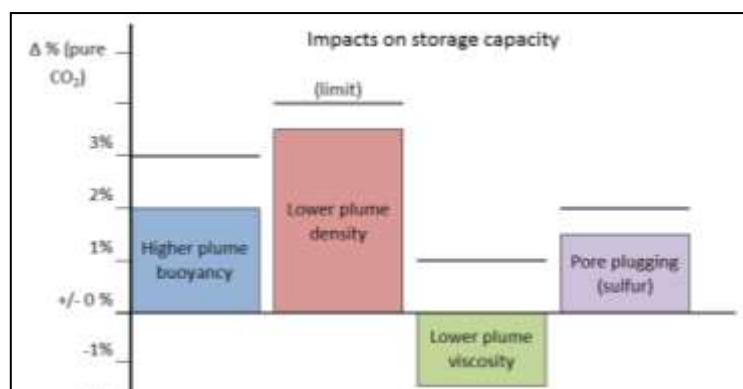

Figure 3: Example of global assessment for a given CO2 stream and for selected parameters

References

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[2] R.Farret, P. Gombert, F. Lahaie, A. Cherkaoui, S. Lafortune, P. Roux ; Design of fault trees as a practical method for risk analysis of CCS: application to the different life stages of deep aquifer storage, combining long-term and short-term issues, Energy Procedia 4, 2011